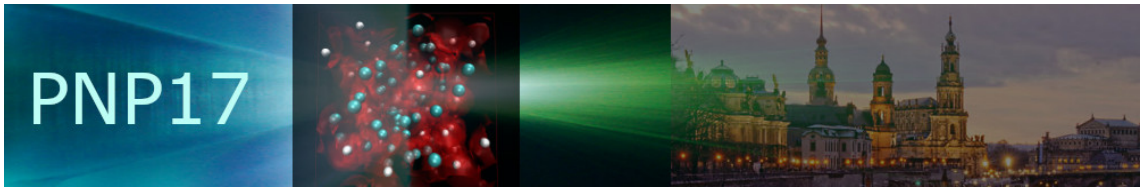

Physics of Nonideal Plasmas 17

September 20th to 24th 2021, Dresden, Germany

September 15, 2021

HZDR HiBEF

Universität Rostock

Welcome Address

Dear Friends and Colleagues, welcome to Dresden! The organisation committee from Helmholtz-Zentrum Dresden-Rossendorf and Universität Rostock is proud to present the

17th Physics of Nonideal Plasmas Conference

to you.

The conference will be held in the very centre of beautiful Dresden, state capital and home to an excellent Technical University. Besides the Helmholtz-Zentrum Dresden-Rossendorf, Dresden is home to four Max-Planck Institutes or centres, ten Fraunhofer Institutes, five Institutes of the Leibniz society, and many more.

Within walking distance from the conference venue in the Hilton hotel, you will find many museums displaying world famous artefacts (see *Grünes Gewölbe*), theatres, architectural masterpieces, parks, the river Elbe running through town, and a whole host of different eating, drinking and shopping possibilities.

We hope that we can convey the spirit of the conference to all online attendees as well. These times are a little different but with the help of modern technology we can still share our work and enthusiasm.

The PNP series of conferences was born in the north-eastern part of Germany when the country was still divided into East and West. It outgrew its original community and remote village locations after the german reunification. We are happy to still welcome members of the original community from Rostock, Greifswald, and Russia. We further welcome everyone who has joined us since then from all over the world and has helped the field of nonideal plasmas, of strongly coupled plasmas, and of warm dense matter research grow and become stronger. We especially welcome everyone who will join us for the first time, be it young student, or seasoned researcher and we hope that you all will not only be having a good time in Dresden and doing science here but will also permanently be with us in the future for the next conference.

We wish all of you an exciting conference and a good time here in Dresden.

The organisation and programme committee

Contents

Overview

	Sunday 19th Sept.	Monday 20th Sept.		Tuesday 21st Sept.		Wednesday 22nd Sept.		Thursday 23rd Sept.		Friday 24th Sept.	
08:50		Opening									
09:00 09:40		Kraus	Bethkenhagen	Clerouin	Kang	Redmer	Mintsev	Tkachenko	Khrapak	Reinholz	Moldabekov
09:40 10:00			Filinov		Chen		Röpke		Soubiran		Yu
10:00 10:20			Cangi		Kim		Tkachenko		Pain		Davletov
10:20 10:40			Blanchet		Fiedler		Issanova		Zaporozhets		Fairushin
10:40-11:10			break		break		break		break		break
11:10 11:30		Vorberger	Zeng	Bethkenhagen	Preising	Neumayer	Zastrau	Sauerbrey	Toncian	Redmer	Brault
11:30 11:50			Bergerman		Ramakrishna		Preston				Martynova
11:50 12:10			Dornheim		Kumar		Smid		Bernert		Sametov
12:10 12:30			Bonitz		Nikolaev		French		Nakatsumi		Closing
12:30 12:50			Redmer		He		Stevenson		Neumayer		
12:50-14:30			lunch		lunch		lunch		lunch		departure
14:30 15:10		Toncian	Ofori-Okai	Bonitz	Starret		Excursion	Zastrau	McBride		
15:10 15:30			Choi		Ceperley				Humphries		
15:30 15:50			White						Hartley		
15:50 16:10			Schoelmerich		Kononov				Silvestri		
16:10-17:00			break		break				break		
17:00 17:20				Cangi	Militzer						
17:20 17:40					Blouin						
17:40 18:00	reception		P1		Graziani				P2		
18:00 18:30											
							Conference Dinner				

Talks in Chronological Order

Density Functional Theory calculations for high-temperature carbon plasmas

Monday
20 Sep
09:00

Mandy Bethkenhagen[1], T. Döppner[2], S. H. Glenzer[3], S. Hamel[2], D. Kraus[4,5], J. E. Pask[2], G. Röpke[4], M. Schörner[4], A. Sharma[6], P. A. Sterne[2], P. Suryanarayana[6], B.B.L. Witte[3,4], R. Redmer[4]

[1]École Normale Supérieure de Lyon, 46 Allée d'Italie, 69364 Lyon, FRANCE
[2]Lawrence Livermore National Laboratory, Livermore, CA 94550, USA
[3]SLAC National Accelerator Laboratory, Menlo Park, CA 94025 USA
[4]University of Rostock, Institute of Physics, 18051 Rostock, GERMANY
[5]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, GERMANY
[6]Georgia Institute of Technology, Atlanta, GA 30332, USA

Accurately modeling warm dense matter deep inside astrophysical objects is a grand challenge. The associated thermodynamic states are characterized by solid-state densities, temperatures of thousands of Kelvin, and GPa pressures. The extreme of the conditions can vary gravely depending on the mass, radius, and composition of the studied object ranging from several GPa in planetary mantles to millions of GPa at the center of stellar interiors. A method that has proven highly successful in describing this peculiar state of matter is density functional theory molecular dynamics (DFT-MD). However, while the equations of states and transport properties for giant planets like Jupiter or Neptune became increasingly accessible with DFT-MD simulations in the last two decades, extreme conditions as predicted for the interiors of brown dwarfs and low-mass stars seemed beyond reach. In this talk, we discuss how DFT-MD calculations can be pushed to millions of Kelvin using carbon as an example. At very high densities, traditional DFT-MD codes based on plane-waves can be still used and we present a new ab initio approach to calculate the ionization degree based on the sum rule for the dynamic electrical conductivity [1]. We find a significantly higher carbon ionization degree than predicted by commonly used models, yet validating the qualitative behavior predicted by average atom models. The results are directly used to model the plasma parameters of ongoing experimental campaigns at the National Ignition Facility aiming at recreating the conditions inside brown dwarfs and low-mass stars. At low densities and high temperatures, however, traditional plane-wave codes become intractable, because the number of partially occupied states increases significantly. This problem is addressed with the novel SQDFT code, which is a large-scale implementation of the Spectral Quadrature (SQ) method for O(N) Kohn-Sham DFT calculations [2,3]. The new capabilities of SQDFT are demonstrated for the Hugoniot curve for carbon

up to 10 million Kelvin.
[1] M. Bethkenhagen, B.B.L. Witte, M. Schörner, G. Röpke, T. Döppner, D. Kraus, S. H. Glenzer, P. A. Sterne, R. Redmer, Physical Review Research 2, 023260 (2020).
[2] P. Suryanarayana, P. P. Pratapa, A. Sharma, and J. E. Pask, Computer Physics Communications 224, 288 (2018).
[3] A. Sharma, S. Hamel, M. Bethkenhagen, J. E. Pask, P. Suryanarayana, Journal of Chemical Physics 153, 034112 (2020).

Fermionic propagator path integral Monte Carlo simulations: Equation-of-state of hydrogen plasma without the fixed-node approximation

Monday
20 Sep
09:40

Alexey Filinov[1,2], Pavel Levashov[1], Michael Bonitz[2]

[1] JIHT RAS, Russia
[2] Kiel University, Kiel, Germany

In recent years a significant progress has been achieved in studying the finite-temperature exchange and correlation effects of the uniform electron gas using the fixed-node QMC [1] and fermionic path integral simulations [2,3]. In the present work we extend the method of anti-symmetrised density matrix [2,3] to the grand-canonical ensemble and perform ab initio simulations of hydrogen plasma down to temperatures 15 000 K including the onset of the transition to molecular phase. The isotherms for the pressure and the internal energy are compared with the Fixed-node PIMC [4] and hydrogen EOS based on DFT-MD [5]. This allows us to conclude on the accuracy of different methods depending on the degeneracy parameter. Furthermore, we derive novel finite size corrections for dense hydrogen which allows to reconstruct an accurate equation of state valid in the thermodynamic limit being important for ICF applications. We also discuss the composition and structure of degenerate quantum plasma in terms of pair correlation functions, the ionic static structure factor and the momentum distribution of electrons[6].
[1] E.W. Brown et al, Phys. Rev. Lett, 110, 146405 (2013)
[2] Siu A Chin, Phys. Rev. E, 031301 (2015)
[3] T. Dornheim, S. Groth et al., Phys.Rep. 744, 1-86 (2018)
[4] S.X. Hu et al, Phys.Rev. B 84, 224109 (2011)
[5] A. Becker et al, Astrophys. Jour. Supp. Series 215, 21 (2014)
[6] K. Hunger et al, Phys. Rev. E (2021) in press (arXiv:2101.00842)
The authors gratefully acknowledge financial support from DFG via project BO1366/15-1 (Germany) and by the grant No. 13.1902.21.0035 (Russia).

Data-driven Multiscale Modeling of Matter under Extreme Conditions

Monday
20 Sep
10:00

Attila Cangi
Center for Advanced Systems Understanding (CASUS) Helmholtz-Zentrum Dresden-Rossendorf

Data-driven Multiscale Modeling of Matter under Extreme Conditions The successful characterization of high energy density (HED) phenomena in laboratories using pulsed power facilities and coherent light sources is possible only with numerical modeling for design, diagnostic development, and data interpretation. The persistence of electron correlation in HED matter is one of the greatest challenges for accurate numerical modeling and has hitherto impeded our ability to model HED phenomena across multiple length and time scales at sufficient accuracy. Standard methods from electronic structure theory capture electron correlation at high accuracy, but are limited to small scales due to their high computational cost. In this talk I will summarize our recent efforts on devising a data-driven workflow to tackle this challenge. Based on first-principles data we generate machine-learning surrogate models that replace traditional electronic-structure algorithms. Our surrogates both predict the electronic structure and yield thermo-magneto-elastic materials properties of matter under extreme conditions highly efficiently while maintaining their accuracy.

Extended-DFT model for high temperatures simulations in ABINIT and application to warm dense aluminum and boron

Monday
20 Sep
10:20

A. Blanchet[1,2], J. Clérouin[1,2], F. Soubiran[1,2] and M. Torrent[1,2]
[1] CEA-DAM-DIF, F-91297 Arpajon, France
[2] Université Paris-Saclay, CEA, Laboratoire Matière sous Conditions Extrêmes, 91680 Bruyères-le-Châtel, France

The extended first-principle molecular dynamics (FPMD) model introduced by Zhang et al. [1], has been implemented within the ab-initio DFT software package ABINIT and is now publicly available [2]. This model allows to perform quantum molecular dynamics simulations (QMD) at high temperature bypassing the well-known orbital wall[3]. QMD simulations can be done smoothly in the full range of temperatures from cold condensed matter to hot plasmas (¿ 10000 eV) passing by the warm dense matter regime. At high temperature, a minimum of Kohn-Sham orbitals is kept allowing for deep ionization effects to manifest, such as the Shottky anomaly, at contrast with orbital-free approaches where this effect is absent. After a reformulation of the model in terms of Gaussian packets and with analytical evaluations of the high energy electron contributions, we present applications to aluminum and boron. Simulations for multiple isochores, from few Kelvins to thousands of eVs, result in Hugoniot transformations very close to the FPEOS model [4], for a much lower computational intensity. The Kubo-Greewood formulation for optical properties in this context is addressed.

[1] S. Zhang, H. Wang, W. Kang, P. Zhang, and X. T. He, "Extended application of Kohn-Sham firstprinciples molecular dynamics method with plane wave approximation at high energy from cold materials to hot dense plasmas," Physics of Plasmas, vol. 23, p. 042707, (2016).
[2] A. Blanchet, J. Clérouin, F. Soubiran and M. Torrent submitted to Computer Physics Communications (2021).
[3] A. Blanchet, M. Torrent, and J. Clérouin, "Requirements for very high temperature Kohn-Sham D¡FT simulations and how to bypass them," Physics of Plasmas, vol. 27, p. 122706, (2020).
[4] B. Militzer, F. Gonzalez-Cataldo, S. Zhang, K. P. Driver, and F. Soubiran, "First-principles equation of state database for warm dense matter computation," Phys. Rev. E, vol. 103, p. 013203, (2021).

Ab Initio Validation on the Connection between Atomistic and Hydrodynamic Description to Unravel the Ion Dynamics of Warm Dense Matter

Monday
20 Sep
11:10

Qiyu Zeng[1], Xiaoxiang Yu[1], Yunpeng Yao[1], Tianyu Gao[1], Bo Chen[1], Shen Zhang[1], Dongdong Kang[1], Han Wang[2], and Jiayu Dai[1]

[1]Department of Physics, National University of Defense Technology, Changsha, 410073, P. R. China

[2]Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing 100088, P. R. China

Ion dynamics contains both atomistic motions and hydrodynamic behaviors, thus exhibit inherent multiscale characteristics. Although atomic-scale ab initio molecular dynamics is a subject of intense research for warm dense matter (WDM), the zero-frequency mode of ion-ion dynamic structure factor (DSF), which contains the information of the onset of relaxation processes, could not be demonstrated within ab initio framework due to the limitation of simulated sizes. Here, we fill this gap by combing microscopic and hydrodynamic descriptions. To capture the ion dynamics near the hydrodynamic limit with ab initio accuracy, an accurate and efficient electron-temperature dependent interatomic potential is constructed via the machine-learning deep potential method. This key step can bridge the atomic scale and hydrodynamic picture, helping us quantitatively verify the consistency of thermal diffusivities obtained from hydrodynamics and fluctuation-dissipation theorem, and providing a new perspective from microscopic dynamics of energy transport to accurately demonstrate the ion dynamics of warm dense matter. We presented specific analysis on the microscopic mechanism behind the damping of the central peak for non-equilibrium warm dense aluminum, and a competitive mechanism between significant hardening of acoustic collective excitations and suppressed self-diffusion of ions is found.

Corresponding author: jydai@nudt.edu.cn

Gibbs-ensemble Monte Carlo simulations for binary mixtures

Monday
20 Sep
11:30

A. Bergermann, M. French, and R. Redmer
Institut für Physik, Universität Rostock, D-18051 Rostock, Germany

We explore the performance of the Gibbs-ensemble Monte Carlo simulation method by calculating the miscibility g
ap of $H_2 - He$ mixtures with analytical exponential-six potentials [1]. We calculate demixing curves for pressures up to 500 kbar and temperatures up to 1800 K. Our results are in good agreement with ab initio simulations in the non-dissociated region of the phase diagram [3]. Next, we determine new parameters for the Stockmayer potential [3] to model the interactions in the $H_2 - H_2O$ system for temperatures of 1000 K<T<2000 K. The corresponding miscibility gap of $H_2 - H_20$ mixtures was determined and we calculated demixing curves for pressures up to 150 kbar and temperatures up to 2000 K. Our results show reasonable agreement with previous experimental data of Bali et al [4]. These results are important for interior and evolution models for ice giant planets because $H_2 - H_20$ demixing would induce compositional gradients which could inhibit convection and, therefore, the cooling of those planets [5, 6].

[1] A. Bergermann, M. French, M. Schöttler and R. Redmer, Phys. Rev. E, 103 (2021)
[2] M. Schöttler and R. Redmer, Phys. Rev. Let. 120, 115703 (2018)
[3] W. Stockmayer, J. Chem. Phys. 9, S. 398-402 (1941)
[4] E. Bali, A. Audétat and H. Keppler, Nature, 495, 7440 (2013)
[5] R. Helled, N. Nettelmann and T. Guillot, Space Sci. Rev., 216 (2020)
[6] E. Bailey and D. J. Stevenson, arXiv, (2. Februar 2021)

Effective Static Approximation: A Fast and Reliable Tool for Warm-Dense Matter Theory

Monday
20 Sep
11:50

Tobias Dornheim
CASUS, HZDR, Görlitz, Germany

Warm dense matter is of high current interest for many applications, including astrophysics, material science, and fusion research. Yet, the accurate description of electronic correlation effects at these conditions is most difficult, and often computationally intensive ab-initio methods have to be used. Here we present the effective static approximation (ESA) [1] to the local field correction (LFC) of the electron gas, which enables highly accurate calculations of electronic properties like the dynamic structure factor $S(q, \omega)$, the static structure factor $S(q)$, and the interaction energy v with no computational extra cost compared to the random phase approximation (RPA). More specifically, the ESA combines the recent neural-net representation of ab-initio path integral Monte Carlo results [2] of the temperature-dependent LFC in the exact static limit with a consistent large wavenumber limit. It is suited for a straightforward integration into existing codes. We demonstrate the importance

of the LFC for practical applications by re-evaluating the recent x-ray Thomson scattering experiment on aluminum by Sperling et al. [3]. We find that an accurate incorporation of electronic correlations within the ESA leads to a different prediction of the inelastic scattering spectrum than obtained from state-of-the-art models like linear-response time-dependent density functional theory. Furthermore, the ESA scheme is particularly relevant for the development of advanced exchangecorrelation functionals in density functional theory, or for the computation of material properties like the thermal/electrical conductivity, stopping power, etc. Finally, the ESA is now readily available as an analytical representation [4] and can be easily incorporated into existing codes.

[1] T. Dornheim et al., Phys. Rev. Lett. 125, 235001 (2020)
[2] T. Dornheim et al., J. Chem. Phys. 151, 194104 (2019)
[3] P. Sperling et al., Phys. Rev. Lett. 115, 115001 (2015)
[4] T. Dornheim et al., Phys. Rev. B 103, 165102 (2021)

Monday
20 Sep
12:10

Momentum distribution function and short-range correlations of electrons in dense quantum plasmas – ab initio quantum Monte Carlo results

M. Bonitz[1], K. Hunger[1], T. Schoof[2], A. Filinov[1], and T. Dornheim[3]

[1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

[2]DESY

[3]CASUS, HZDR, Görlitz, Germany

In a classical plasma the momentum distribution, n(k), decays exponentially, for large k, and the same is observed for an ideal Fermi gas. However, when quantum and correlation effects are relevant simultaneously, an algebraic decay, $n_\infty(k) \sim 1/k^8$ has been predicted. This is of relevance for cross sections and threshold processes in dense plasmas that depend on the number of energetic particles. Here we present the first ab initio results for the momentum distribution of the nonideal uniform electron gas in the entire warm dense matter range. Our results are based on first principle fermionic path integral Monte Carlo (PIMC) simulations and clearly confirm the $1/k^8$ asymptotic. This aymptotic behavior is directly linked to short-range correlations which are analyzed via the on-top pair distribution function (on-top PDF). We present extensive accurate results for the density and temperature dependence of the on-top PDF and for the momentum distribution in the entire momentum range. At the end, we extend the results to twocomponent quantum plasmas. For the case of dense hydrogen we investigate, via ab initio fermionic PIMC simulations [2], the influence of electron-proton correlations and the formation of atoms and molecules on the momentum distribution. This work is supported by the Deutsche Forschungsgemeinschaft via grant BO1366/15.

[1] K. Hunger et al., Phys. Rev. E, in press
[2] A. Filinov and M. Bonitz, submitted for publication

Collective x-ray Thomson scattering for conditions inside brown dwarfs using the National Ignition Facility

Monday
20 Sep
12:30

R. Redmer[1], M. Schörner[1], M. Bethkenhagen[1,2], B. B. L. Witte[1], D. Kraus[1,3], L. B. Fletcher[4], S. H. Glenzer[4], P. Neumayer[5], M. J. MacDonald[6], L. Divol[6], O. L. Landen[6], J. Kline[6], A. Yi[6], T. Döppner[6]

[1]University of Rostock, Institute of Physics, D-18051 Rostock, GERMANY
[2]ENS Lyon, Laboratoire de Géologie de Lyon, Lyon 69364, FRANCE
[3]Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, GERMANY
[4]SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA
[5]GSI Helmholtz-Zentrum für Schwerionenforschung, D-64291 Darmstadt, GERMANY
[6]Lawrence Livermore National Laboratory, Livermore, CA 94550, USA

Brown dwarfs lie in the mass range 13 MJ *le* MBD $\leq$ 75 MJ between massive giant planets and the smallest red dwarf stars; MJ being the Jupiter mass. In their interior extreme conditions of densities up to several hundred g/cm3 and temperatures up to 200 eV are predicted [1] and indications for a strong magnetic field are found [2]. The explanation of the dynamo action in BDs requires precise EOS data and conductivities for such extreme conditions that have never been probed simultaneously in a laboratory experiment up to now. Therefore, we have performed inelastic scattering experiments at the National Ignition Facility in forward scatter geometry in order to determine the temperature for conditions deep inside BDs from first principles via detailed balance [3] and the electrical conductivity from the plasmon collisional damping [4]. This was enabled by performing high-resolution x-ray scattering experiments using a spectrally narrow 9 keV x-ray probe on hohlraum-driven compressed targets [5]. The scattering spectra were analyzed by comparing with first-principles DFT-MD simulations that include scattering contributions of bound and free electrons and a self-consistent calculation of the ionization state. For the first time, electrical conductivities are measured for the extreme conditions as found in the deep interior of BDs.

[1] A. Becker et al., Astrophys. J. Suppl. Ser. 215, 21 (2014).
[2] S.V. Beryudina et al., Astrophys. J. 847, 61 (2017).
[3] S.H. Glenzer, R. Redmer, Rev. Mod. Phys. 81, 1625 (2009).
[4] M. Bethkenhagen et al., Phys. Rev. Research 2, 023260 (2020).
[5] M.J. MacDonald et al., Phys. Plasmas 28, 032708 (2021).

We acknowledge the NIF Discovery Science program for providing access to the facility. This work was supported by the DFG via the Research Unit FOR 2440. The DFT-MD simulations were performed at the North-German Supercomputing Alliance (HLRN) and at the IT and Media Center of the University of Rostock.

Monday
20 Sep
14:30

Measuring the near-DC electrical conductivity of warm dense matter using THz spectroscopy

Benjamin Ofori-Okai
LCLS, SLAC, Stanford, USA

The DC electrical conductivity is an important parameter for characterizing warm dense matter and dense plasmas as it is connected with carrier density and electron-electron and electron-ion collisional processes. Accurate knowledge is vital, for instance, for modeling the magnetic field produced by planetary dynamos, or for understanding instability growth in inertial confinement fusion implosions. However, investigations of the DC conductivity have remained a significant challenge due to the highly transient nature of laboratory generated warm dense matter. Probing transient states on ultrashort time scales is possible using ultrafast laser pulses, but these approaches measure the high frequency AC response. Information extracted from these measurements must then be extrapolated to the lowfrequency near-DC regime. Additionally, theoretical models predict different results based on how the strong coupling of dense plasmas is handled. Taken together, these highlight the need for accurate measurements of the response close to DC. Ultrafast terahertz (THz) radiation has emerged as a useful tool for investigating materials and have been used in many scientific areas. One advantage is that THz fields are slowly time-varying, appearing essentially static relative to the time scale of electron and ion interactions relevant for measuring properties like the electrical conductivity. This alone makes THz spectroscopy incisive, but additionally, single-cycle THz pulses can sub-picosecond in duration. Consequently, time-resolved THz spectroscopy directly captures information about DC-like material properties using an ultrafast probe. This cannot be attained with pulses at lower, i.e. gigahertz, frequencies, but is critical for characterizing highly transient states such as laboratory generated warm dense matter. This talk presents recent measurements of the DC electrical conductivity of warm dense matter using terahertz (THz) pulses. The THz pulses are produced using laser- or accelerator-based techniques and measured with high-fidelity single-shot electro-optic sampling. Using a pump-probe measurement, the electrical conductivity of warm dense matter produced by femtosecond laser heating is determined with ¡ 1 ps temporal resolution. The measurements demonstrate the influence of material density and changes in the collision frequency on the electrical conductivity, and our results are compared with density functional theory calculations of warm dense aluminum. Lastly, the talk will present an outlook on using THz pulses for studies of dynamically compressed matter and show initial results in which THz measurements are combined with structural measurements using diffraction which characterize the warm dense matter state produced.

Influence of Dissipation and Effective Interaction on the Dense Plasma Dynamic Structure Factor

Monday 20 Sep 15:10

Yongjun Choi[1] and Michael S. Murillo[2]

[1]Institute for Cyber-Enabled Research, Michigan State University, East Lansing, Michigan 48824, USA

[2]Computational Mathematics, Science and Engineering, Michigan State University, East Lansing, Michigan 48824, USA

The ionic dynamic structure factor is examined to assess the relative roles of dissipation and the effective ionic interaction. Two disparate physically based models of dissipation, which can differ numerically by orders of magnitude, are used in molecular dynamics. We find a negligible impact on the amplitudes of the dynamic structure factors for physically realistic parameter values. We then examine the effective ionic interaction by varying its strength, the size of the atomic core (through a pseudopotential) and the screening model. We find that "diffusive" peaks in the dynamic structure factor are very sensitive to the form of the ionic interaction, and this sensitivity arises primarily from atomic physics through the pseudopotential. This suggests that it would be useful to employ the measured zero-frequency dynamic structure factor $S_{ii}(k, 0)$ as a constraint on the effective interaction, which in turn can be used to compute physical properties.

Measuring Transport Properties in Warm Dense Matter with Fresnel Refractive Diffractive Radiography

Monday 20 Sep 15:30

T. G. White[1], C. H. Allen[1], M. Oliver[2], L. Divol[3], Z. Karmiol[1], A. Kemp[3], O. L. Landen[3], Y. Ping[3], M. Schoelmerich[3], W. Theobald[4], and T. Döppner[3]

[1]University of Nevada, Reno, NV, USA

[2]Central Laser Facility, Rutherford Appleton Laboratory, UK

[3]Lawrence Livermore National Laboratory, Livermore, CA, USA

[4]Laboratory for Laser Energetics, Rochester, NY, USA

Thermal conductivity and particle diffusion play a vital role in several areas of contemporary warm dense matter (WDM) research, including astrophysical and inertial confinement fusion (ICF) systems. However, significant variations in predictions and a scarcity of experimental measurements hamper our understanding [1]. We present an overview of the development of our Fresnel Refractive Diffractive Radiography (FDR) platform for the Omega and NIF laser facilities. This platform couples isochorically heated buried wires with dynamic X-ray phasecontrast imaging [2]. By utilizing novel 1 µm-wide slits, five times smaller than previously demonstrated, we obtain a highly spatially coherent x-ray source that gives rise to significant refractive and diffractive features from micron-scale density gradients at the interface [3]. Measurement of the evolution of this density profile, driven primarily by particle diffusivity and thermal conductivity, opens the door for direct measurements of transport properties in WDM [4]. We will present successful imaging of dynamic WDM systems at Omega and provide details on future experiments planned for NIF, which will measure the evolution of the interface between CH and

liquid D2 samples.
[1] P.E. Grabowski et al. High Energy Density Physics, 37, 100905 (2020).
[2] A. Pogany, D. Gao, and S. W. Wilkins. Review of Scientific Instruments 68, 2774-2782 (1997).
[3] E. L. Dewald et al. Review of Scientific Instruments 89, 10G108 (2018).
[4] Y. Ping et al. Journal of Instrumentation 6, P09004 (2011).
The work of Y.P., L.D., O.L., M.S. and T.D. was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC5207NA27344 and supported by Laboratory Directed Research and Development (LDRD) Grant No. 21-ERD-029. The work of C.H.A and T.G.W. was supported by the National Science Foundation under grant no. 2045718.
Corresponding Author Email: tgwhite@unr.edu

Monday
20 Sep
15:50

SiO_2 shock melt- and release experiments at LCLS and SACLA

M.O. Schoelmerich[1,2] , T. Tschentscher[2] , C. A. Bolme[3], E. Cunningham[3], E. Galtier[4], A.E. Gleason[4], M. Harmand[5], Y. Inubushi[6,7], K. Katagari[8], K. Myzanishi[6], B. Nagler[4], N. Ozaki[8], T.R. Preston[2], R. Redmer[9], R.F. Smith[1], T. Togashi[6,7], S.J. Tracy[10], Y. Umeda[8], L. Wollenweber[2], T. Yabuuchi[6,7], U. Zastrau[2], K. Appel[2]

[1]Lawrence Livermore National Laboratory, Livermore, USA
[2]European XFEL, Schenefeld, Germany
[3]Los Alamos National Laboratory, Los Alamos, USA
[4]SLAC National Accelerator Laboratory, Menlo Park, USA
[5]Institute of Mineralogy, Materials Physics and Cosmochemistry, Paris, France
[6]RIKEN SPring-8 Center, Sayo-cho, Sayo-gun, Hyogo, Japan
[7]Japan Synchrotron Radiation Research Institute, Sayo-cho, Sayo-gun, Hyogo, Japan
[8]Osaka University, Suita, Osaka, Japan
[9]Universität Rostock, Institut für Physik, Rostock, Germany
[10]Earth and Planets Laboratory, Carnegie Institution of Washington, Washington D.C., USA

Melting properties of planetary materials, such as silica, play an essential role in planetary dynamics, and its equilibrium properties and melting behavior might have a direct impact on the electromagnetic field around Earth [1]. It is therefore of great interest to investigate silicate melts on the atomic scale at pressures corresponding to lower mantle conditions ($>$ 1 Mbar). Furthermore, recrystallization effects from melts can constrain pressure and temperature conditions of other geophysical events, such as meteor impacts. We therefore conducted a series of shock compression experiments to elucidate the melt- and shock release behavior of SiO_2 on the lattice level. The experiments were carried out at the Matter in Extreme Conditions (MEC)and the BL3:EH5 end-stations of the LCLS and SACLA X-ray free electron laser (XFEL). Samples were compressed to pressures of up to 159(13) GPa and subsequently probed by hard X-rays (11.2 keV and 11 keV, respectively). Timing of the X-rays was set according to the peak compression of the sample (close

to the shock breakout) and at late time delays of up to 250 ns after laser impact. The scattering signal of the melt and the released samples allow to gain information about the respective amorphization or solidification at decreasing pressures and temperatures. Results were compared to DFT-MD simulations and give important constrains on the bonding behavior of silicates at extreme conditions.

[1] B. A. Remington, R. E. Rudd, and J. S. Wark, Physics of Plasmas 22, 090501 (2015).

Corresponding Author Email: schoelmerich1@llnl.gov

Equation of states and atomic structures of matter under extreme conditions and the extension to large scale by machine learning

Tuesday
21 Sep
09:00

Dongdong Kang, Bo Chen, Qiyu Zeng, Yong Hou, Jiayu Dai

Department of Physics, National University of Defense Technology, Changsha, Hunan 410073, P. R. China

Although the study of EOS is an old topic, there is a longstanding lack of global accurate EOS data of matter (DT mixtures, silicon, et al.) under extreme conditions within a unified theoretical framework. The biggest challenge for obtaining accurate EOS data with first-principles methods is the treatment of electron–ion interactions and the extremely high computational cost at high temperatures and large scale. We performed extensive state-of-the-art ab initio quantum Langevin molecular dynamics simulations to obtain EOS data of DT mixtures for ICF conditions. The EOS data of silicon and several typical metals were also calculated. The solidsolid and liquid-liquid phase transition of these materials were systematically investigated. We extended the first-principles calculations to high-temperature and large-scale by using deep potential molecular dynamics simulations, where the potential is generated by deep neutral network trained with ab initio data. In addition, we introduce a scheme for predicting electronic density of state (DOS) in large scale molecular dynamics simulations, within the framework of deep neutral network. We show that the proposed scheme provides an efficient and accurate protocol on time-resolved and spatial-resolved analysis of electron structures in dynamic process of warm dense matter. References [1] Jiayu Dai, Yong Hou, and Jianmin Yuan, Phys. Rev. Lett. 104, 245001 (2010)
[2] Jiayu Dai, Dongdong Kang, Zengxiu Zhao, Yanqun Wu, and Jianmin Yuan, Phys. Rev. Lett. 109, 175701 (2012)
[3] Binbin Lu, Dongdong Kang, Dan Wang, Tianyu Gao, and Jiayu Dai, Chin. Phys. Lett. 36, 103102 (2019)
[4] Dongdong Kang, Yong Hou, Qiyu Zeng, and Jiayu Dai. Matter Radiat. Extremes, 5, 055401 (2020).
[5] Dongdong Kang, Kai Luo, K. Runge et al., Matter Radiat. Extremes, 5, 064403 (2020).
[6] Qiyu Zeng et al. Unpublished.
ddkang@nudt.edu.cn, jydai@nudt.edu.cn

Atomic-scale study on the dynamics of structural transformation under shock compression

Tuesday
21 Sep
09:40

Bo Chen[1], Qiyu Zeng[1], Han Wang[2], Dongdong Kang[1], Jiayu Dai[1], Andrew Ng[3]

[1]Department of Physics, National University of Defense Technology, Changsha 410073, P. R. China

[2]Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing 100088, P. R. China

[3]Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T-1Z1, Canada

Shock compression is a common technology to obtain high pressure-temperature environments, for discovering and predicting novel states and materials under the extreme conditions found in giant-planet interiors. Elucidating the microscopic mechanism of structural transformation of many shock-compressed materials is much demanded and full of challenges. By using molecular dynamics simulations, the structural transformation processes of facecentered cubic (FCC) gold and polyethylene under shock compressions have been unambiguously revealed from the atomic level. In agreement with recent experiments, the sequence of structures, stacking faults, body-centered cubic (BCC) phase, and coexistence of BCC-amorphous phase are found until gold reaching completely melting up to 325 GPa. A much lower FCC-BCC transition pressure (112GPa for ¡100¿ and 220GPa for ¡110¿) is observed compared to static compression. It is because the shock-induced BCC structures accompany with more atomic disorders than perfect crystal, reducing the free energies and consequently largely lowering the transition pressure [1]. For shock-compressed polyethylene to conditions around 125 GPa and 4,500 K, the phase separation of hydrocarbons into diamond and hydrogen has been found. In the process of demixing, polyethylene firstly cracked into small molecules such as hydrogen, methane, and ethane, and the remaining carbon atoms begin to be enriched into amorphous carbon. And then these carbon atoms crystallized into diamond as they aggregated. The crystallization of diamond grows spontaneously only when the critical nucleation radius is reached, conforming to the classical nucleation theory. These simulations revealed the dynamics structural transformation of shock-compressed materials and help to provide more further understanding of such observations also in experiments [2-4]. Corresponding author: J. Dai, jydai@nudt.edu.cn. [1] B. Chen, Q. Zeng, H. Wang, D. Kang, J. Dai, and A. Ng, (arXiv e-prints 2020), pp. arXiv:2006.13136
[2] R. Briggs, F. Coppari, M. G. Gorman, R. F. Smith, S. J. Tracy, A. L. Coleman, A. FernandezPanella, M. Millot, J. H. Eggert, and D. E. Fratanduono, Phys. Rev. Lett. 123, 045701 (2019).
[3] S. M. Sharma, S. J. Turneaure, J. M. Winey, Y. Li, P. Rigg, A. Schuman, N. Sinclair, Y. Toyoda, X. Wang, N. Weir, J. Zhang, and Y. M. Gupta, Phys. Rev. Lett. 123, 045702 (2019).
[4] D. Kraus, J. Vorberger, A. Pak, N. J. Hartley, L. B. Fletcher, S. Frydrych, E. Galtier, E. J. Gamboa, D. O. Gericke, and S. H. Glenzer, Nature Astronomy 1, 606 (2017).

Hydrodynamic simulation of the future HED matter EOS research experiments at FAIR

Tuesday
21 Sep
10:00

V.V. Kim, D.N. Nikolaev, I.V. Lomonosov, V.B. Mintsev
IPCP RAS, Chernogolovka, Russia

New ion beam experiments cycle for HED matter properties and EOS research is scheduled at FAIR facility. Based on previous HIHEX (Heavy Ion Heating and EXpansion) experiment results held at GSI [1] it was proposed to use the focused heavy ion beam for fast and uniform heating of thin metallic (Lead) foil, that melts, evaporates and expands to the sides in quasy-1-D regime. In order to reach closer

to the main area of interest on the metal phase diagram - critical point (CP) and evaporation curve - it was supposed to use enclosing high-pressure assembly, filled with heavy transparent gas (Ar, initial pressure 100 bar). The shock wave generated in Ar by hot expanding Lead creates counter-pressure up to few kilobars, while remaining transparent. It allows one to use different registration and diagnostic techniques: pyrometry, interferometry, reflectivity measurement, shadowgraphy and schlieren shadowgraphy. From the announced list of feasible projectile beam configurations on the 2021 FAIR operation we chose U, Ni, Ar and N ion beams as the most promising for our goals, realistic intensities estimated for these beams were selected. Bunch duration is 100 ns with parabolic temporal distribution. Considering the geometry of the lead specimen 2-D Gaussian distribution for spatial beam focal spot was used, with fixed Sigmax=0.25 mm and varying Sigmay=0.5-1.5 mm. Staying in that range preserves high enough energy deposition value as well as quasy-1-D hydrodynamic flow regime even at the later stages of experiment. Multidimensional hydrodynamic implementation of finite size particle-in-cell method was used for 1and 2-D modelling. SRIM-based ion stopping procedure was used for heavy ion beam energy deposition effect in the Pb-target and ambient Ar gas, using tabular wide-range multiphase equation of state for Lead [3]. The history of Pb-target material parameters were recorded during the numerical experiment. It was found that in order to get to near-critical point region states in Lead during expansion phase of the experiment the peak projected specific internal energy values in the target should be higher than 1 kJ/g. Thus only the usage of Ni ion beam with up to 1.E+11 particles looks appropriate and N, Ar and U beams with lower intensities are not sufficient. In order to estimate the level of intensity needed for the U ion beam, we simulate the impact of increased values of I=3.0E+09 and I=4.0E+09 particles/bunch. It was shown that for highly focused U beam with I=3.0E+09 the parameters in Lead in expansion phase of the experiment are at a lower end of the main area of interest, and higher beam energetic parameters are desirable.

[1] D. Varentsov et al., Nucl. Instr. & Meth. in Phys. Res. A. 577(1-2) (2007) 262-266
[2] V.E. Fortov et al., Int. J. Impact Eng. 33 (2006) 244
[3] V.E. Fortov et al., Nucl. Instr. & Meth. in Phys. Res. A. 415, 3 (1998) 604-608

Tuesday
21 Sep
10:20

Materials Learning Algorithms (MALA): An Efficient Surrogate for Ab-initio Simulations

Lenz Fiedler
CASUS, Görlitz, Germany

Ab-initio simulations are useful for many scientific applications, from materials science to drug discovery. This is due to powerful simulation techniques such as Density Functional Theory (DFT) that combine high accuracy with computational feasibility. Yet, there exist applications unattainable with even the most performant DFT codes. A prominent example is the modeling of materials on multiple time and length scales, especially under ambient and extreme conditions. While these simulations

hold the potential to both further our understanding of important physical phenomena such as planetary formation and radiation damage in fusion reactor walls, they evade traditional ab-initio approaches due to their size and complexity. Surrogate models can mitigate these computational restrictions, by reproducing DFT-level results at a fraction of the cost. Here, were present the Materials Learning Algorithms (MALA) package, an open source python package for building neural-network-based surrogate models for materials science. MALA provides easy-to-use functions to process DFT data and build machine-learning models that replace DFT calculations. We illustrate simulations for solid and liquid aluminium and liquid iron at 3000 K. The source code for MALA is publicly available on Github and is developed by the Center for Advanced Systems Understanding (CASUS), Sandia National Laboratories, and Oak Ridge National Laboratory.

Metallization of dense fluid helium from ab initio simulations

Tuesday
21 Sep
11:10

Martin Preising, Ronald Redmer
Universität Rostock, Rostock, Germany

An earlier study [1] benchmarked Density Functional Theory (DFT) coupled with classical Molecular Dynamics (MD) with all available experimental data on dense helium in recent years. A subsequent study [2] calculated the helium melting line with DFT-MD. These two studies allows for the examination of the metallization of fluid helium consistently with DFTMD. We study the insulator-to-metal transition at densities between 1 and 22 g/cm^3 and temperatures between 10 000 and 50 000 K. We calculate the equation of state, the band gap dependent on density and temperature by using different definitions [3-6], the DC conductivity, the reflectivity, and the ionization degree for which a novel method has been proposed recently [see M. Bethkenhagen et al., Phys. Rev. Res. 2, 023260 (2020)]. We find no indication of a first-order phase transition in any of the properties studied here and conclude that the metallization of fluid helium is continuous. For instance, we do not observe jumps in the DC conductivity and/or the reflectivity when the band gap closes. However, the ionization degree increases from below 10% at the lowest to over 99% at the highest densities which reflects the continuous insulator-to-metal transition. The increase is almost exclusively driven by pressure ionization and shows only a weak temperature dependence. We discuss the high-pressure phase diagram of helium and the implications of our results on the structure of astrophysical objects like gas giant planets and brown dwarfs.

[1] Preising et al., Equation of state and optical properties of warm dense helium, Phys. Plasmas 25, 012706 (2018).
[2] Preising et al., High-pressure melting line of helium from ab initio calculations, Phys. Rev. B. 100, 184107 (2019).
[3] Kowalski et al., Equation of state and optical properties of warm dense helium, Proc. Rev. B 76, 11071 (2007).
[4] Stixrude et al., Fluid helium at conditions of giant planetary interiors, Proc. Natl. Acad. Sci. USA 32, 11071 (2008).

[5] Monserrat et al., Fluid helium at conditions of giant planetary interiors, Phys. Rev. Lett. 112, 055504 (2014).
[6] W. Zhang et al., Revisiting metallization boundary of warm dense helium in a wide ρ-T regime from ab initio study, Sci. Rep. 7, 41885 (2017).

Electrical conductivity of Iron under Earth core conditions using time-dependent density functional theory

Tuesday 21 Sep 11:30

Kushal Ramakrishna, Jan Vorberger, Attila Cangi
Helmholtz-Zentrum Dresden-Rossendorf (HZDR), D-01328 Dresden, Germany

Iron is one of the most plentiful components on the planet earth and plays a crucial role in our lives. The analysis of iron at high pressures and temperatures is of great geophysical importance because iron makes up the majority of the Earth's liquid outer core and solid inner core. The technical utility of iron is due to the large phase space of iron-based alloys, which is the source of a wide range of steel microstructures that can be produced with minor compositional changes and proper thermal treatment. The iron phase structure at the extreme conditions under the inner core conditions of the earth is still not conclusive especially in the vicinity of temperature around 6000 K and pressures nearing 300 GPa. Time-dependent density functional theory (TDDFT) enables calculating electronic transport properties in warm dense matter (WDM) and is an alternative to present state-of-the-art approaches. In TDDFT, the electrical conductivity is computed from the time evolution of the electronic current density and provides direct means to assess the validity of Ohm's law in WDM. We present TDDFT calculations of the electrical conductivity for iron within the pressure and temperature range found in Earth's core. We discuss the ramifications of using TDDFT for calculating the electrical conductivity in contrast to the Kubo-Greenwood formalism and dielectric models.

Ionization and transport in partially ionized multi-component plasmas: Plasma model for Hot Jupiter atmospheres

Tuesday 21 Sep 11:50

Sandeep Kumar, Anna Julia Poser, Manuel Schöttler, Uwe Kleinschmidt, Martin French, and Ronald Redmer
Institute for Physics, University of Rostock, D-18051, Rostock, Germany

Profound knowledge of ionization and transport of multi-componet plasmas is important for applications in astrophysics, atmospheric science, and plasma technology. In this work, we study ionization and transport processes in the multi-component plasma of Hot Jupiter atmospheres. Mass-action laws are used to calculate the composition of the plasma and electron-ion and electron-neutral transport cross-sections. Based on the plasma composition and these cross-sections, the electrical conductivity, thermal conductivity, and Lorenz number is calculated. The effect of electron-electron scattering on the transport properties is considered via a correction

factor to the electron-ion contribution. For the thermal conductivity, we consider also the contributions of the translational motion of neutral particles and of the dissociation, ionization, and recombination reactions. The characteristics of ionization and transport with varying mass density and temperature of the plasma are investigated in detail. The profiles of ionization and transport properties along typical pressure-temperature profiles of the outer part of the Hot Jupiter HD 209458b are also studied. Our results are important for the study of Ohmic dissipation processes in Hot Jupiter and hot mini-Neptunes.

Dense Silicon Plasma Emission under Pressures 70-510 GPa

Tuesday
21 Sep
12:10

D.N.Nikolaev, M.I.Kulish, S.V.Dudin. V.B.Mintsev, I.V.Lomonosov, V.E.Fortov

Institute of Problems of Chemical Physics RAS, 142432, Chernogolovka, Russia

Monocrystalline silicon has a transparency window in the infrared region (1.2 - 8 microns). Photoreceivers for spectral region of 0.9 - 2.6 microns, based on indium-gallium arsenide are available. This make possible to register the thermal radiation from the shock wave front in silicon by an optical pyrometry technique, previously used to measure the temperature of shock compressed transparent substances in the visible range of spectra. Shock compression of single-crystal Silicon up to pressure 70 - 130 GPa was realized using the launching of flyer plates by explosive detonation; explosive Mach-type cumulative generators allowed to achieve pressures up to 510 GPa. Silicon shock Hugoniot was determined by precise measurement of wave velocities in monocrystalline quartz reference and Silicon with optical technique and impedance matching. To measure the brightness temperatures of the shock wave front, a four-channel infrared optical pyrometer with a fiber input of radiation was designed. Registration bands, centered at wavelengths 1.3, 1.5, 1.6, and 1.8 μm were used. Shock compressibility data, obtained at 280 – 510 GPa range, demonstrates significantly soft Hugoniot in comparison with Pavlovsky's data at 80-196 GPa in 1968, and good match with laser experiment by Henderson in 2021. The optical emission of shock front in silicon and brightness temperature in the infrared transparency window of spectrum were measured. The effect of opacity of the elastic shock wave precursor front in silicon at 70 GPa was confirmed. The significant difference of experimental and calculated temperature (2 -5 times lower) was found at pressures of 200-510 GPa. A similar phenomenon was observed in the experiments by Lower in 1998. Appearance of the electronhole plasma layer before shock wave front due to the thermal conductivity and photoionization process not allows to describe this phenomena. Analysis of the kinetics of ionization and formation of the electron concentration gradient at shock front gives the estimation of the ionization rate and gradient layer thickness, which prove to be of the order of $\sim 2 \cdot 10^9$ s^{-1} and $\sim 10\mu$m correspondingly.

Tuesday
21 Sep
12:30

Diamond formation kinetics in shock-compressed $C-H-O$ samples via small angle X-ray scattering

Z. He[1,2], J. Lütgert[1], J. Vorberger[1], M.G. Stevenson[2], L.M.V. Zinta[2], B. Heuser[2], O. Humphries[1], A.K. Schuster[1], K. Voigt[1], D. Ranjan[2], M. Bethkenhagen[3], M. French[2], A. Bergmann[2], R. Redmer[1], T.E. Cowan[1], T. Vinci[4], E.E. McBride[5], N.J. Hartley[5], A.E. Gleason-Holbrook[5], S.H. Glenzer[5], S. Pandolfi[5], B. Nagler[5], H.J. Lee[5], E. Galtier[5], D. Khaghani[5], A. Descamps[5], B. Ofori-Okai[5], C. Schoenwaelder[5], C. Glen[5], J.-A. Hernandez[6], A. Ravasio[4], D. Kraus[1,2]

[1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany.
[2]Universität Rostock, Rostock, Germany.
[3]ENS, Lyon, France.
[4]Laboratoire LULI, Ecole Polytechnique, Palaiseau, France.
[5]SLAC National Accelerator Laboratory, Menlo Park, USA.
[6]University of Oslo, Oslo, Norway

Icy giant planets such as Neptune and Uranus are abundant in our galaxy. The interiors of these celestial objects are thought to be mainly composed of a dense fluid mixture of water, methane and ammonia [1]. Due to the high pressure and high temperature conditions deep inside the planet, this material mixture will likely undergo chemical reactions and structural transitions[2]. An example of these reactions is the possible dissociation of hydrocarbons, and subsequent phase separation, allowing the formation of diamonds. Laser shock experiments in combination with an XFEL allowed us to address these questions.[3-5] Due to the presence of water and therefore large amounts of oxygen inside the ice giants, investigating C-H-O samples provides a more realistic scenario than studying pure hydrocarbon systems. As an ultra-sensitive diagnostic technique, small angle X-ray scattering (SAXS)[6] can explore feature sizes in the order of nanometers by recording their scattering at small angles (typically 0.1-10°), allowing us to obtain deeper insights into the question how diamonds are formed, what grain sizes are achieved and how many grains are formed. Experiments were carried out at the MEC end station of the LCLS XFEL in December 2020. Three oxygenated polymers with different carbon to H_2O ratios, polyethylene terephthalate (PET, $C_{10}H_8O_4$), polylactic acid (PLA, $C_3H_4O_2$) and cellulose acetate (CA, $C_{10}H_{16}O_8$) were compressed to planetary interior states ranging from 50 GPa to 150 GPa and 2000 K to 7000 K by laser-driven single shocks. The compressed samples were probed utilizing in situ X-ray diffraction (XRD) and SAXS. The diamond formation kinetics in presence of oxygen in these three materials have been observed. SAXS shows more sensitive information than XRD, revealing that the diamond fraction first increases and then decreases with increasing of pressure and the growth of particles with time in the medium pressure regime (∼110 GPa). The observed particle radius of diamond is between 1.5 nm and 3 nm. In addition, the proportion of carbon in the initial sample materials also shows a correlation with the observed diamond fraction. Ongoing simulations aim to explain these phenomena in order to improve the theory of planetary formation and evolution.

[1]T. Guillot, Annu. Rev. Earth Planet. Sci. 33, (2005).
[2]M. Ross, Nature 292, (1981).
[3]D. Kraus, J. Vorberger, A. Pak, et al., Nature Astronomy 1, (2017).

[4]D. Kraus, N. Hartley, S. Frydrych, et al., Phys. Plasmas 25, (2018).
[5]A. Schuster, N. Hartley, J. Vorberger, et al., Phys. Rev. B 101, (2020).
[6]O. Glatter, O. Kratky and H. Kratky, Small angle X-ray scattering (Academic press, 1982).
email: zhiyu.he@uni-rostock.de
Use of the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515. The MEC instrument is supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences under Contract No. SF00515. This work was supported by the Helmholtz Association under VH-NG-1141 and ERC-RA-0041.

Multi-Center Calculations of the Equation-of-state of Carbon at Very High Pressures

Tuesday
21 Sep
14:30

Charles Starrett , Crystal Ottoway, Didier Saumon
Los Alamos National Laboratory

Accurate knowledge of the equation of state of carbon at megabar to gigabar pressures is important for white dwarf simulation. However, it is very challenging to include all relevant physics in models that predict equation of state. Here we present calculations using a newly developed multiple scattering method for warm and hot dense matter. We will give an overview of this method, which includes the physics of partial ionization, ionic disorder and electron degeneracy, and is based on finite temperature density functional theory. We will also present results on the principal Hugoniot to very high pressures, and compare to other methods.

Electronic energy gap closure and metal-insulator transition in dense liquid hydrogen

Tuesday
21 Sep
15:10

David Ceperley
University of Illinois at Urbana-Champaign, Illinois,USA

We develop a method for calculating the fundamental electronic gap of semiconductors and insulators using grand canonical quantum Monte Carlo (QMC) simulations. We discuss the origin of the bias introduced by supercell calculations of finite size and show how to correct the leading and subleading finite size errors either based on observables accessible in the finite-sized simulations or from density-functional theory calculations. Using these QMC calculations, we investigate the insulator-metal transition observed in liquid hydrogen at high pressure. Below the critical temperature of the transition from the molecular to the atomic liquid, the fundamental electronic gap closure occurs abruptly, with a small discontinuity reflecting the weak first-order transition in the thermodynamic equation of state. Above the critical temperature, molecular dissociation sets in while the gap is still open. When the gap closes, the decay of the off-diagonal reduced density matrix shows that the

liquid enters a gapless, but localized phase: there is a cross-over between the insulating and the metallic liquids. Compared to different DFT functionals, our QMC calculations provide larger values for the fundamental gap and the electronic density of states close to the band edges, indicating that optical properties from DFT potentially benefit from error cancellations. We also study the gap closure with pressure of crystalline molecular hydrogen. Nuclear zero point effects cause a large reduction in the gap (2eV). Depending on the structure, the fundamental indirect gap closes between 380GPa and 530GPa for ideal crystals and 330-380GPa for quantum crystals. Beyond this pressure the system enters into a bad metal phase where the density of states at the Fermi level increases with pressure up to 450-500 GPa when the direct gap closes. Our work partially supports the interpretation of recent experiments in high pressure hydrogen

---

Tuesday
21 Sep
15:50

Bound-bound features in x-ray Thomson scattering signals

Alina Kononov[1] , Thomas Hentschel[2] , Andrew D. Baczewski[1], Stephanie B. Hansen[3]

[1] Center for Computing Research, Sandia National Laboratories, Albuquerque NM, USA
[2] School of Applied & Engineering Physics, Cornell University, Ithaca NY, USA
[3] Pulsed Power Sciences Center, Sandia National Laboratories, Albuquerque NM, USA

Warm dense matter (WDM) experiments rely on diagnostic techniques such as x-ray Thomson scattering, where plasmonic features in the inelastic scattering spectrum are sensitive to electronic temperature. Typical approaches to thermometry are based on the application of detailed balance to red- and blue-shifted plasmons, but various sources of uncertainties pose challenges for this method. We propose peaks arising from bound-bound transitions, i.e., scattering into thermally depleted core orbitals, as alternative diagnostic features which we predict to become increasingly prominent at high temperatures. For the cases of iron and aluminum isochorically heated to 1eV and 20eV, our first-principles, real-time timedependent density functional theory calculations validate an average atom model modified to treat d-band electrons as quasibound states. This work lays the foundation for accurate diagnostic tools as higher temperatures become accessible on XFEL platforms. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

First-Principles Equation of State (FPEOS) Database And Dilute Cores in Giant Planets

Tuesday
21 Sep
17:00

Burkhard Militzer
University of California, Berkeley

This talk will discuss two equation of state applications. First, we will describe a first-principles equation of state (FPEOS) database for matter at extreme conditions that we put together by combining results from path integral Monte Carlo and density functional molecular dynamics simulations of eleven elements and ten compounds [1]. For all these materials, pressure and internal energy are provided over a wide density-temperature range from 0.5 to 50 g/cc and from 10^5 to 10^9 K. Results from 5000 first-principles simulations were combined. In this talk, we focus on isobars, adiabats and shock Hugoniot curves of different silicates in the regime of L and K shell ionization. Second, we will discuss how uncertainties in the equation of state of hydrogen-helium mixtures affect our understanding of giant planets. We will review the gravity measurements of the Juno spacecraft that has been in orbit about Jupiter since 2016. Interpreting these measurements has been a challenge because it is difficult to reconcile the unexpectedly small magnitudes of the moments J4 and J6 with conventional interior models that assume an ab initio equations of state as well as a compact core of ice and rock. We conclude by discussing models for Jupiter's interior that include cores that have been substantially diluted with hydrogen and helium.

[1] B. Militzer, F. Gonzalez-Cataldo, S. Zhang, K. P. Driver, F. Soubiran, First-principles equation of state database for warm dense matter computation, Phys. Rev. E 103 (2021) 013203. DOI: 10.1103/PhysRevE.103.013203

FPEOS webpage: http://militzer.berkeley.edu/FPEOS

Direct Evaluation of the Phase Diagrams of Dense Multicomponent Plasmas by Integration of the Clapeyron Equations

Tuesday
21 Sep
17:20

Simon Blouin, Jerome Daligault, and Didier Saumon
Los Alamos National Laboratory

When a multicomponent plasma freezes, the coexisting liquid and solid phases generally have different compositions. This fractionation has important consequences for the modeling of dense stellar plasmas, such as those found in white dwarf stars. To quantify the fractionation process, the phase diagram of the relevant plasma mixture is required. Such phase diagrams have been computed using a variety of standard techniques, which suffer from physical and computational limitations. I will present a new Monte Carlo-based approach that we have recently developed to accurately and efficiently obtain the phase diagrams of dense plasmas (arXiv:2104.00599, to appear in Phys. Rev. E). The method is an adaptation of the Gibbs-Duhem integration approach to electron-ion plasmas, where the liquid-solid coexistence curve is determined by direct numerical integration of its underlying Clapeyron equation.

We have applied this new technique with great success to problems relevant to the interiors of white dwarf stars (Astron. Astrophys., 640, L11 and Astrophys. J. Lett., 911, L5), and many other applications are within its scope.

Tuesday
21 Sep
17:40

Quantum hydrodynamics and shock physics

Frank Graziani
ITAP, Kiel University, Germany

Shocks exist in a wide variety of solid, fluid, and gas phenomena. Of particular interest for a wide range of high energy density science experiments are shocks produced at extreme conditions such as in warm dense matter during the implosion of inertially confined fusion capsules or equation of state experiments. We use quantum hydrodynamics (QHD) with Fermi pressure, Bohm pressure, exchange, Poisson, and viscosity contributions to better understand shock propagation and shock structure in degenerate matter. We compare and contrast the shock physics described by QHD with that of classical fluid equations.

Vladimir E.Fortov and Non-Ideal Plasma Physics

Wednesday
22 Sep
09:00

V.B.Mintsev

Institute of Problems of Chemical Physics, Chernogolovka, Moscow Reg., 142432 Russia

This report is devoted to the history of VE Fortov's scientific research in the field of physics of non-ideal plasma generated by dynamic methods - the main and most beloved scientific problem in his life. He starts this activity like a student, postgraduate Student of the Moscow Institute of Physics and Technology of the Department of the Research Center named after Keldysh under leadership of professor VM Ievlev. His first works deal with the non-ideal cesium plasma, generated in preheated shock tube. In 1971 starts his scientific work in Chernogolovka in the Institute of Chemical Physics. Here VE Fortov carried out research on generation, study of the physical properties and gas dynamics of dense low-temperature plasma, which then develops into a new scientific direction - Physics of extreme states of matter and dynamic processes at high energy densities. A non-ideal plasma becomes the main object, when the average Coulomb interaction energy turns out to be of the same order of magnitude as the average kinetic energy. Its generation is carried out by powerful shock waves generated by the high explosives. Intensive experimental and theoretical studies of the compressibility, electrical conductivity, optical properties of such a medium are published in a number of central Russian journals and the first books on the physics of non-ideal plasma were out in print. International cooperation is developing rapidly, of which I especially note the cooperation with German scientists from the Universities of Berlin, Rostock, Greifswald and GSI Helmholtzzentrum für Schwerionenforschung in Darmstadt. Experiments carried out at the end of the 90s to study the electrophysical properties of shock-compressed plasma testified to the appearance of a high level of electrical conductivity (corresponding to a metallic one) in hydrogen and noble gases at high densities in the region of megabar pressures. This process of plasma "metallization" has found its explanation in the framework of the pressure ionization process due to strong Coulomb interaction. And the determination of the quasiisentropical compressibility of deuterium in joint experiments with VNIIEF made it possible for the first time to speak on the discovery of a special first-order phase transition at a pressure of ∼140 GPa - a plasma phase transition. VE Fortov and his collaborators showed particular interest in processing the latest experiments of VNIIEF to achieve record pressures of ∼20 TPa in the plasma of deuterium and helium and to create new equations of state in this exotic range of parameters. In recent years, VE Fortov has been doing a lot of physics of astrophysical objects and quark-gluon plasma, where the effects of strong interaction are especially pronounced. In particular, the analysis of the limiting expression for the ratio of shear viscosity to specific entropy, derived within the framework of modern string theory, showed that a non-ideal plasma with a strong Coulomb interaction is an example of such a medium, so that in this sense it can be called a perfect liquid. VE Fortov was always full of scientific ideas. Unfortunately, not all ideas were implemented. But he left behind a large school of his followers, among whom there are many young people. I hope they continue to penetrate into this extremely interesting area of science – Physics of non-ideal plasma.

Equation of State of Hydrogen, Helium and Plasmas in the Sun

Wednesday
22 Sep
09:40

Werner Ebeling[1], Heidi Reinholz[2], Gerd Röpke[2]

[1] Institute of Physics, Humboldt University, Berlin, Germany
[2] Institute of Physics, Rostock University, Rostock, Germany

The equation of state (EoS) of plasmas of the two lightest elements H and He, and of mixtures as typical for the plasmas in the sun are calculated. The contributions of deep bound states are included by using inverted fugacity expansions. The inversion of fugacities to densities is reduced to solvable algebraic problems.The calculation of relative pressures is done separately for low and for high densities. Near the crossing point, in between, the separate solutions are connected to each other by smooth concatenation at the crossing points. Applications to hydrogen - helium plasmas in the sun are discussed including calculations of the adiabatic EoS.

Static and dynamic properties of classical and quantum one-component plasmas

Wednesday
22 Sep
10:00

J. Ara, Ll. Coloma, I.M. Tkachenko

Universitat Politècnica de València, Spain

The dynamic structure factor and other dynamic characteristics of strongly coupled onecomponent plasmas are studied using the self-consistent version of the method of moments [1]. The advantage of this approach is that the dynamic characteristics are expressed in terms of the static ones (the static structure factor) without any adjustment to the simulation data and taking the energy dissipation processes into account. A semiquantitative agreement is achieved with recent simulation data on Coulomb and Yukawa systems including the data on the dynamic local-field correction function [2]. Agreement can be improved if the uncertainties in the static characteristics are accounted for. In addition, the static dielectric function and other static characteristics of dense warm charged Fermi liquids are also obtained exclusively from the system static structure factor. These results are in quantitative agreement with the numerical data obtained recently by the path-integral Monte-Carlo method [3]. Alternative theoretical approaches including the standard and extended random-phase approximations are employed as well. Perspectives of the method are outlined.

[1] Yu. V. Arkhipov et al., Phys. Rev. Lett. 119, 045001 (2017).
[2] Yu. V. Arkhipov et al., Phys. Rev. E 102, 053215 (2020).
[3] P. Hamann et al., Phys. Rev. B 102, 125150 (2020) and references therein.

Ion core effect on scattering processes in dense plasmas

Wednesday
22 Sep
10:20

Ramazanov T.S., Kodanova S.K., Issanova M.K.

IETP, Al-Farabi Kazakh National University, Almaty, Kazakhstan, Al-Farabi av., 71

Among the plasma diversity, a non-ideal dense plasma is particularly difficult object to study due to the presence of strong inter-particle correlations and quantum degeneracy effects in the system. Understanding of prop-erties of a non-ideal dense plasma with a high concentration of heavy ions is important for modern astrophysics [1, 3, 5, 6]. In addition, such a plasma is created in con-trolled thermonuclear fusion experiments [1–4].The method of effective potentials is one of the often-used approaches to compute structural, transport and thermodynamic properties of plasmas [7]. We note that the fundamental difference between this work and research conducted in the world is that the effective potentials proposed by the take into account collective screening at large distances due to weakly bound electrons and ions with a small charge, and strongly correlated heavy ions, as well as the quantum-mechanical effects of diffraction and symmetry at small distances due to partial quantum degeneracy of electrons. Moreover, along with the above characteristics, the project will also take into account the core effect (finite size) of heavy ions, which is important for describing electron scattering by a heavy ion. In this work the impact of the of the ion core effect on the scattering phase shifts, the partial (total) cross-section, and transport cross-section due to modification of the screening were considered. The results obtained for the scattering processes are compared with the results of the Born approximation with the data obtained in terms of classical scattering of particles interacting by the Yukawa potential.

[1] Fortov V.E. Extreme States of Matter in High Energy Density Physics. – Springer, 2016.

[2] Sharkov B.Yu., Hoffmann D.H.H., Golubev A.A., and Zhao Y. Matter Radiat. Extremes. – 2016. – Vol. 1. – P. 28-47.

[3] Graziani F., Desjarlais M.P., Redmer R. and Trickey S.B. Frontiers and challenges in warm dense matter. – Springer, 2014.

[4] Hoffmann D.H.H., Blazevic A., Rosmej O., Roth M., Tahir N.A., Tauschwitz A., Udrea A., Varentsov D., Weyrich K., and Maron Y. Laser Part. Beams. – 2005. – Vol. 23. – P. 47-53.

[5] Moldabekov Zh.A., Groth S., Dornheim T., Kählert H., Bonitz M., and Ramazanov T.S. Phys. Rev. E. – 2018. – Vol. 98. – P. 023207.

[6] Haensel P., Potekhin A.Y., Yakovlev D.G. Neutron Stars 1: Equation of State and Structure. – Springer, 2007.

[7] Issanova M.K., Kodanova S.K., Ramazanov T.S., Bastykova N.Kh., Moldabekov Zh.A., and Meister C.-V. Laser and Particle Beams (2016), 34, 457–466.

issanova@physics.kz

Wednesday
22 Sep
11:10

HED science at European XFEL – an overview

U. Zastrau[1], K. Appel[1], M. Banjafar[1,2], E. Brambrink[1], C. Baehtz[2], V. Cerantola[1], S. Göde[1], H. Hoeppner[2], J. Kaa[1], Z. Konôpková[1], M. Makita[1], M. Nakatsutsumi[1], A. Pelka[2], C. Prescher[3], C. Plueckthun[1], T. Preston[1], J.-P. Schwinkendorf[1], C. Strohm[3], T. Toncian[2], L. Wollenweber[1]

[1] European XFEL, Schenefeld, Germany, ulf.zastrau@xfel.eu [2] Helmholtz-Zentrum Dresden-Rossendorf HZDR, Dresden, Germany [3]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany

The advent of the first X-ray free-electron lasers (XFELs), FLASH in 2004 and LCLS in 2009, may prove to be the most profound development since the invention of the laser and, equally, the synchrotron. Sharp improvements in a number of laser parameters, most notably intensity and pulse duration, support this expectation. This brings scientific dreams within reach. Indeed, the unprecedented opportunities and expectations have triggered considerable research activities worldwide. The talk will yield an overview of the experimental application of today's XFELs to explore warm dense matter and materials in extreme conditions with advanced time-resolved x-ray methods. Since May 2019, the High Energy Density Science (HED) instrument at the European X-ray FreeElectron Laser Facility in Schenefeld, Germany, allows international users to investigate a wide range of materials and systems at extreme conditions. For sample excitation a variety of high energy drivers are available [1]. In particular, three separate optical laser systems are available for warm- to hot-densematter creation, dynamic compression and laser-plasma interaction in electron-relativistic regime. These drivers allow studying various phase space parameters with time-resolution down to 10 fs, pressures into the TPa regime, and electric field strength up to 10 20 W/cm. This unique instrument is designed to enable the application of various x-ray probes including spectroscopic, diffraction and imaging methods [2]. Also, it is the first XFEL instrument offering a dedicated platform for research in dynamic diamond anvil cells for studies at high pressures. It operates in the photon energy range from 5 to 25 keV and features a variety of platforms facilitating the usage of different techniques in userdriven experiments. The capabilities of the HED instrument, including the HIBEF user consortium contributions [3], will be presented along with selected science cases and first scientific results from the first 2.5 years of user operation [4-6].

[1] M. Nakatsutsumi, et al., Technical design report: Scientific instrument High Energy Density Physics (HED), XFEL:EU TR-2014-001, Germany, 196 p (2014). doi:10.3204/XFEL.EU/TR-2014001. See also www.xfel.eu/research/instruments/hed
[2] K. Appel, et al., Plasma Phys. Control. Fusion 57, 014003 (2015).
[3] www.hibef.de; McMahon and Zastrau, DOI: 10.22003/XFEL.EU-TR-2017-001
[4] A. Descamps et al., Sci Rep 10 (1), 14564 (2020)
[5] H. Hwang et al.; Journal of Physical Chemistry Letters, 2021;
DOI: 10.1021/acs.jpclett.1c00150
[6] H.-P. Liermann et al.; Journal of Synchrotron Radiation, 2021;
DOI: 0.1107/S1600577521002551

New frontiers in X-ray heating with FELs

Wednesday
22 Sep
11:30

T. R. Preston and U. Zastrau

European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany

Since the turn of the 21st century a number of XUV and X-ray Free-electron Lasers, such as FLASH (2004), LCLS (2009), SACLA (2011), and European XFEL (2017) have seen first light. The combination of ultra-short (¡100 fs) pulses and high intensities (¿1017 Wcm-2) on target have revolutionised the creation of uniform solid-density plasmas. Through tuning the photon energy from XUV to X-rays and beyond, high absorption of materials can be achieved by probing around atomic edges and resonances. The energy is then deposited in the material faster than hydrodynamic expansion leading to degenerate, highly-coupled plasmas. These exotic plasmas can be diagnosed by a variety of well-established techniques such as x-ray [1, 2] or electron [3] emission spectroscopy, x-ray Thomson scattering [4] or by ex-situ analysis of imprints [5]. The plasmas provide a test-bed of atomic physics and allow measurements of continuum lowering [6], x-ray lasing [7], opacity [8], atomic rates [9], as well as thermodynamic [10], optical [11], and transport properties [12] of matter, amongst others. New avenues have also been opened up in simulation of warm-dense matter [13, 14]. In this talk the emergent field of x-ray heating will be introduced and its impact on modern measurements will be presented through selected science cases over the last twenty years.

[1] Zastrau et al., PRE 78 066406 (2008)
[2] Vinko et al., Nature 482 59-62 (2012)
[3] Young et al., Nature 466, 56-61 (2010)
[4] Glenzer and Redmer, Rev. Mod. Phys. 81, 1625 (2009)
[5] Chalupský et al., Opt. Express 18, 27836 (2010)
[6] Ciricosta et al., Phys. Rev. Lett. 109, 065002 (2012)
[7] Yoneda et al., Nature 524, 446-449 (2015)
[8] Preston et al., Phys. Rev. Lett. 119, 085001 (2017)
[9] Van den Berg et al., Phys. Rev. Lett. 120, 055002 (2018)
[10] Lee et al., Phys. Rev. Lett. 102, 115001 (2009)
[11] Sperling et al., J. Phys. B: At., Mol. Opt. Phys. 50, 134002 (2017)
[12] Witte et al., Phys. Rev. Lett. 118, 1 (2017)
[13] Son et al., Phys. Rev. X 4, 031004 (2014)
[14] Vinko et al., Nat Commun 5, 3533 (2015)

Email: thomas.preston@xfel.eu

Ultrafast melting of Warm Dense Cu studied by x-ray spectroscopy

Wednesday 22 Sep 11:50

Michal Šmíd, Alexander Köhler, Yen-Yu Chang, J. P. Couperus Cabadağ, Thomas Kurz, Xiayun Pan, Pablo Perez-Martín, Susanne Schöbel, Jan Vorberger, Thomas E. Cowan, Ulrich Schramm, Arie Irman, and Katerina Falk

Helmholtz Zentrum Dresden-Rossendorf, Dresden, Germany

We present a study of ultra fast heating of Warm Dense Cu diagnosed by means of x-ray absorption and emission spectroscopy carried at the Draco laser facility at HZDR. A thin Cu foil is directly heated to few eV temperature by an ultra short laser pulse (40 fs, 1 J) and probed with variable delay in the ps range by a laser-driven betatron radiation. This betatron radiation, created by a laser wakefield accelerator, is an unique x-ray source with its ultra short duration and broadband spectrum, therefore it is ideally suited for studies of non-equilibrium dense plasmas with this diagnostic. The high brightness achieved at Draco can allow for single-shot measurement. The sample is studied via the X-ray absorption spectroscopy in the region above the Cu K-edge and a line emission of the K_β. This method provides temporally-resolved information about both the ionic structure of the matter and its temperature during the process of ultrafast heating and melting of the material.

E-mail: m.smid@hzdr.de

Thermal and optical properties of synthetic planetary HCNO mixtures from ab initio simulations

Wednesday 22 Sep 12:10

Martin French

Universität Rostock, Rostock, Germany

The interiors of the water-ammonia-methane-rich planets Uranus and Neptune are assumed to contain mixtures of these molecular substances with a stoichiometric ratio of C:N:O=4:1:7. While we already have a decent understanding of the physical properties of the individual substances water, ammonia, and methane at high-pressure and high-temperature conditions, much less is known about their mixtures. Recent shock-wave experiments [1] have used water-ethanol-ammonia mixtures with similar stoichiometries as noted above and measured their thermodynamic and optical properties along the Hugoniot curve. The results indicated that such mixtures achieve very similar Hugoniot conditions to those of pure water but show notably different optical reflectivities. Here we perform ab initio simulations based on density functional theory to calculate the Hugoniot curve and the optical properties of synthetic planetary mixtures as used in the experiment [1]. We will discuss the differences to the results for pure water and those from a linear mixing EOS model for water, ammonia, and methane [2]. Changes in structural and chemical properties of the simulated mixtures along the Hugoniot curve will be examined as well. Our results are of high importance for understanding the behavior of multi-component nonideal plasmas under shock compression. The findings are relevant for the development of structural and evolution models for giant planets like Uranus and Neptune

as well as exoplanets of similar composition [3].
[1] M. Guarguaglini, J.-A. Hernandez, T. Okuchi, P. Barroso, A. Benuzzi-Mounaix, M. Bethkenhagen, R. Bolis, E. Brambrink, M. French, Y. Fujimoto, R. Kodama, M. Koenig, F. Lefevre, K. Miyanishi, N. Ozaki, R. Redmer, T. Sano, Y. Umeda, T. Vinci, A. Ravasio, "Laser-driven shock compression of "synthetic planetary mixtures" of water, ethanol, and ammonia", Sci. Rep. 9, 10155 (2019).
[2] M. Bethkenhagen, E. R. Meyer, S. Hamel, N. Nettelmann, M. French, L. Scheibe, C. Ticknor, L. A. Collins, J. D. Kress, J. J. Fortney , and R. Redmer, "Planetary Ices and the Linear Mixing Approximation", Astrophys. J. 848, 67 (2017).
[3] E. Bailey, D. J. Stevenson, "Thermodynamically Governed Interior Models of Uranus and Neptune", Planet. Sci. J. 2, 64 (2021).
This work is supported by the DFG within the FOR 2440 "Matter under Planetary Interior Conditions - High Pressure, Planetary, and Plasma Physics."

Phase Changes in Dynamically Compressed Water

Wednesday
22 Sep
12:30

M. G. Stevenson[1], L.M.V. Zinta[1], B. Heuser[1], Z. He[1], D. Ranjan[1], M. Bethkenhagen[1], M. French[1], A. Bergermann[1], R. Redmer[1], T.E. Cowan[2], O. Humphries[2], J. Lütgert[2], K. Voigt[2], A.K. Schuster[2], F. Lefevre[3], T. Vinci[3], E.E. McBride[4], N.J. Hartley[4], A.E. GleasonHolbrook[4], S.H. Glenzer[4], S. Pandolfi[4], A. Descamps[4], B. Ofori-Okai[4], C. Schoenwaelder[4], C. Glen[4], L.B. Fletcher[4], J. Hernandez[5], A. Ravasio[3], D. Kraus[1,2]

[1] Universität Rostock, Rostock, Germany.
[2] Helmholtz-Zentrum Dresden-Rosendorf, Dresden, Germany.
[3] Laboratoire LULI, Ecole Polytechnique, Palaiseau, France. 4SLAC
[4] National Accelerator Laboratory, Menlo Park, USA.
[5] University of Oslo, Oslo, Norway

Extreme conditions are ubiquitous in nature. Much of the matter in the universe exists under high pressures and temperatures. Of interest, are the planetary interiors of the icy giants, Uranus and Neptune. Which have particularly complex magnetic fields [1]. To understand these complex magnetic fields the conditions and composition of icy giant planetary interiors need to be determined. The interiors of these planets are understood to contain mixtures of water, ammonia and hydrocarbons [2]. Under compression the phase diagram of ice is rather complex. With several phases determined and predicted under high pressure and temperature conditions [3]. High pressure ice above 1500K and 50 GPa is predicted to undergo a superionic transition, where the hydrogen atoms diffuse into the oxygen sublattice [4,5]. These superionic phases are a possible source of the complex magnetic fields of both Uranus and Neptune. Several high-pressure phases of water have been observed in the superionic region of the phase diagram. A body-centred cubic (bcc) phase, which if superionic would be analogous to ice X structure and with increasing pressure a phase transition to a face centred cubic (fcc) phase has been reported [5]. Experiments carried out at the MEC end station at the LCLS XFEL in December 2020, utilised reverberating shocks to compress water into Off-Hugoniot states within the superionic region of the ice phase diagram [6]. Liquid water samples were

confined between a diamond ablator and a rear window, reaching P-T states ranging from 40 GPa and 1200K to 200 GPa and 4000K. The bcc phase of ice has been observed from 50 GPa and 1200 K. A mixed phase region starting at 90 GPa and 2500 K, has been of observed with the bcc phase and a second phase. With increasing pressure the second phase becomes more prominent with the loss of the initial bcc phase.

The higher-pressure ice initially appears to be the fcc phase as described by Millot et al. However, further examination of the diffraction revealed misfits to the fcc lattice and a lack of refinement has suggested that that this may in fact be a different structure. The structure of this phase has yet to be determined. However, several candidates are proposed from predicted high pressure ices [7]. Ongoing work aims to determine these structures of ice under superionic P-T conditions and with comparison with simulation, understand the magnetic field behaviour of icy giant type planets. Acknowledgements: The work was supported by the Helmholtz Association under VH-NG1141 and ERC-RA-0041. Use of the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515. The MEC instrument is supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences under Contract No. SF00515.

[1] W.J. Nellis, J. Phys.: Conf. Ser. 950, 042046 (2017)
[2] M. D. Hofstadter et al., Ice Giants: PreDecadal Survey Mission Study Report, NASA-JPL report JPL-D-100520 (2017)
[3] C. G. Salzmann, J. Chem. Phys 150, 06091 (2019)
[4] I. A. Ryzhkin, Sol. Stat. Com. 56, 1 (1985)
[5] M. Millot et al., Nat. 569, 7755 (2019)
[6] M. Millot et al., Nat. Phys. 14, 3 (2018)
[7] A. Hermann et al., PNAS 109, 3 (2012)
email: michael.stevenson@uni-rostock.de

Vibrational model of thermal conductivity in strongly coupled plasma-related fluids

Thursday 23 Sep 09:00

Sergey Khrapak[1,2]

[1]Joint Institute for High Temperatures, Russian Academy of Sciences, 125412 Moscow, Russia

[2]Research Group on Complex Plasma, German Aerospace Center (DLR), 82234 Wessling, Germany

A simple vibrational model of heat transfer in liquids with soft pairwise interatomic interactions is discussed [1]. A general expression is derived, which involves averaging over the liquid collective mode excitation spectrum. The model is applied to quantify heat transfer in strongly coupled plasma-related fluids such as a three-dimensional one-component plasma and single component Yukawa fluids. Good agreement with existing numerical results is observed. The applicability of the model is not limited to plasma-related systems, it applies for instance to dense Lennard-Jones liquids. Remarkable agreement with the available numerical results is documented also in this case. The model can be easily generalized to heat conduction in twodimensional systems. Although the problem of transport processes in two-dimensional systems remains a controversial issues, some comments related to heat conduction in twodimensional complex (dusty) plasma layers are presented [2]. Limitations of the model are discussed.

[1] S. Khrapak, Vibrational model of thermal conduction in fluids with soft interactions. Phys. Rev. E 103, 013207 (2021).

[2] S. Khrapak, Thermal conduction in two-dimensional complex plasma layers. Phys. Plasmas 28, 010704 (2021).

Electrical conductivity and optical properties of hydrogen-helium mixtures in the megabar regime

Thursday 23 Sep 09:40

Francois Soubiran

CEA DAM-DIF, 91297 Arpajon, France

The spacecrafts Cassini and Juno have provided exquisite data regarding the internal structure of our gas giant planets Saturn and Jupiter. The gravity data indicated for instance that the envelope of these planets is definitely non uniform and has a variable helium to hydrogen ratio with depth. If the exact composition is yet out of reach because of a large uncertainty on the hydrogen-helium phase diagram, the trend is clear. Both have an enrichment in helium above the megabar level and a helium depletion at lower pressure. For Jupiter a diffuse core may be partially mixed with the helium rich region. For Saturn, the demixing is so pronounced that a nearly pure helium layer is expected in the deepest regions of the planet. But the spacecrafts have also sent back beautiful data regarding the magnetic field. To model the dynamo processes at play it is crucial to have the proper conductivity data of the hydrogen and helium mixtures for different compositions. Here, we report a large series of density functional theory (DFT) based calculations of the electronic properties of hydrogen and helium mixtures under a large range

of thermodynamic conditions relevant for the interior of giant planets. Using linear response theory we determined the conductivity of the mixtures. A simple isobaric isothermal ideal mixing rule, although relatively robust regarding the equation of state of these mixtures, is not satisfactory when applied to the electronic properties. It is thus necessary to carefully consider the mixing effects. We will also discuss how the optical properties may advantageously be used in shock experiments to expose the demixing of hydrogen and helium.

Thursday
23 Sep
10:00

A consistent approach for electrical resistivity within Ziman's formalism: from solid state to hot dense plasma

N. Wetta and J.-C. Pain

CEA, DAM, DIF, F-91297 Arpajon, France

The approach presented here allows a consistent calculation of electrical conductivity of dense matter from the solid to the hot plasma using the same procedure [1], consisting in dropping elastic scattering contributions to solid's and liquid's structure factors in the framework of Ziman's theory. The solid's structure factor is computed using a multiphonon expansion; the elastic part (zero-phonon term) corresponds to Bragg peaks, thermally damped by Debye-Waller attenuation factors. For the liquid, a similar elastic contribution to the structure factor results from a long-range order persisting during the characteristic electron-ion scattering time. All the quantities required for the calculation of the resistivities are obtained from our average-atom model, including the total hypernetted-chain structure factor used from the liquid state to the plasma. No interpolation between two limiting structure factors is required. We derive the correction to apply to the resistivity in order to account for the transient long-range order in the liquid and show that it improves considerably the agreement with quantum-molecular dynamics simulations and experimental aluminum's isochoric and isobaric conductivities. Our results suggest that the long-range order in liquid aluminum could be a slightly compressed fcc one. Two series of ultrafast experiments performed on aluminum are also considered, the first one by Milchberg et al. using short laser pulses [2] and the second one by Sperling et al. involving x-ray heating and carried out on the Linac Coherent Light Source facility [3]. Our attempts to explain the latter assuming an initial liquid state at an ion temperature much smaller than the electron one suggest that the actual initial state before main heating is neither perfectly solid nor a normal liquid.

[1] N. Wetta and J.-C. Pain, Phys. Rev. E 102, 053209 (2020).
[2] H. M. Milchberg et al.,Phys.Rev.Lett. 61, 2364 (1988).
[3] P. Sperling et al.,Phys.Rev.Lett. 115, 115001 (2015).

Warm dense matter explored with shock wave experiments

Thursday 23 Sep 10:20

Yuri Zaporozhets

Institute of Problems of Chemical Physics of the Russian Academy of Sciences, Academician Semenov Avenue 1, Chernogolovka, Moscow Region 142432, RUSSIA

The analysis of the response of a dense plasma to the action of an electromagnetic wave is an important cornerstone for the construction of theoretical models describing warm dense matter and can be used as a tool for investigating the validity of these models. The results of a study of the optical properties of a strongly correlated plasma in the near-infrared and green spectral regions at a plasma mass density $\rho = 0.82$ g/cm^3 are presented. The plasma was investigated by the method of oblique sensing at a wide range of exposure angles. The composition and thermodynamic parameters of the plasma were determined using the modified Saha IV code [1, 2]. The spatial parameters of the plasma transition layer are determined based on the numerical solution of the field equations. Estimates of the viscosity coefficient of the plasma under study are given.

[1] Fortov V E, Gryaznov V K, Mintsev V B, Ternovoi V Ya, Iosilevskiy I L, Zhernokletov M V and Mochalov M A 2001 Contrib. Plasma Phys. 41 215.

[2] Gryaznov V K, Iosilevskiy I L and Fortov V E 2012 AIP Conf. Proc. 917 1426.

The authors acknowledge financial support by DFG-RFBR Grant No. 19-52-12039.

ReLaX: the HiBEF high-intensity short-pulse laser driver at the HED instrument at EuXFEL, its properties and first user experimental results

Thursday 23 Sep 11:10

Toma Toncian

HIBEF consortium

High-energy and high-intensity lasers are essential for pushing the boundaries of science. Their development has allowed leaps forward in basic research areas including laser-plasma interaction, high-energy density science, metrology, biology and medical technology. The HiBEF user consortium contributes and operates two high-peak-power optical lasers at the HED instrument of the European XFEL facility. These lasers will be used to generate transient extreme states of density and temperature to be probed by the X-Ray beam. This contribution introduces the ReLaX laser, a short-pulse high-intensity Ti:Sa laser system, and discusses its characteristics as available for user experiments. As the outcome of internal commissioning experiments we will as show unprecedented synchronization results for a 100 TW class laser and will validate the performance as laser-plasma driver with relativistic I ¿ 10^{20} W/cm^2 intensity on target by investigations of TNSA as laser-proton acceleration mechanism. Additionally we have investigated the effect of EMP and laser generated secondary radiation and particle sources on several x-ray diagnostics, and have developed successful strategies to reduce their impacts. The commissioning of ReLaX is concluded by the successful run of the first user experiment “HED 2621: User community assisted commissioning of the UHI Laser at HED, impact of relativistic

plasma environment on x-ray diagnostics". The main goal of 2621 was to validate SAXS, PCI and x-ray spectroscopy on a variety of targets covering a multitude of science cases such as, hole boring, relativistic transparency, fast electron transport along extended target, isochoric heating of buried targets, EOS determination by shocked targets, plasma instabilities in relativistic intensity regime.

High intensity laser interaction with solid-density cryogenic hydrogen jet targets

Thursday
23 Sep
11:50

C. Bernert[1,2], S. Assenbaum[1,2], F.-E. Brack[1,2], Th.E. Cowan[1,2], C.B. Curry[3,4], F. Fiuza[3], M. Garten[1,2], L. Gaus[1,2], M. Gauthier[3], S. Göde[5], I. Goethel[1,2], S.H. Glenzer[3], A. Huebl[1,6], J.B. Kim[3], Th. Kluge[1], S. Kraft[1], F. Kroll[1], J. Metzkes-Ng[1], M. Loeser[1], L. Obst-Huebl[1,6], M. Rehwald[1,2], M. Reimold[1,2], H.-P. Schlenvoigt[1], C. Schoenwaelder[3,7], U. Schramm[1,2], M. Siebold[1], F. Treffert[3,8], T. Ziegler[1,2], K. Zeil[1]

[1] Helmholtz-Zentrum Dresden – Rossendorf (HZDR), 01328 Dresden, Germany
[2] Technische Universitaet Dresden, 01069 Dresden, Germany
[3] SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA
[4] University of Alberta, Edmonton, Alberta T6G 1H9, Canada
[5] European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Germany [6] Present address: Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA
[7] Friedrich-Alexander Universität Erlangen-Nürnberg, 91054 Erlangen, Germany
[8] Technical University Darmstadt, 64289 Darmstadt, Germany

Ultra-intense short-pulse lasers in the Petawatt regime and intensity range of 10^{21}W/cm^2 offer the possibility to study new compact accelerator schemes by utilizing solid density targets for the generation of energetic ion beams. The optimization of the acceleration process demands comprehensive exploration of the involved plasma dynamics. This applies not only on the femtosecond but also on the pico- to nanosecond timescale, where the laser rising edge modifies the target prior to the 30 fs laser peak. Cryogenic hydrogen jet targets with µm-scale transverse size and solid density (5.2x1022 cm-3) offer the superb opportunity for renewable and debris-free acceleration sources and at the same time allow for comprehensive experimental investigation and realistic simulation of the rich physics involved in the laser target interaction [1]. Here, we present the results of an experiment for laser proton acceleration from a cryogenic hydrogen jet target at the DRACO-PW laser. Optimized acceleration performance is achieved by tailoring the targets plasma density via hydrodynamic expansion induced by a short low-intensity pre-pulse. Optical shadowgraphy probing is utilized to give a realistic input of the targets plasma density for 3 dimensional particle-in-cell simulations of the particle acceleration process.
[1] L. Obst et al. Efficient laser-driven proton acceleration from cylindrical and planar cryogenic hydrogen jets. Sci. Rep., 7:10248, 2017.
E-mail : c.bernert@hzdr.de

Nanoscale subsurface dynamics of solids by grazing-incidence xray scattering with an intense laser

Thursday
23 Sep
12:10

M. Nakatsutsumi[1,10], L. Randolph[2], M. Banjafar[1,3], J-P. Schwinkendorf[1], T. R. Preston[1], T. Yabuuchi[4,5], M. Makita[1], N. P. Dover[6], C. Bähtz[3], E. Brambrink[1], Z. Chen[7], B-I. Cho[8], S. Glenzer[7], S. Göde[1], H. Höppner[3], L. Huang[3], Y. Inubushi[4,5], G. Jakob[9], J. Kaa[1], A. Kon[6], J. K. Koga[6], D. Ksenzov[2], T. Matsuoka[10,11], M. Nishiuchi[6], M. Paulus[12], A. Pelka[3], V. Recoules[13], Ch. Rödel[14], F. Schon[2], K. Sueda[5], Y. Sentoku[11,15], T. Togashi[4,5], T. Toncian[3], L. Wollenweber[1], M. Bussmann[3], T. E. Cowan[3], M. Kläui[9], C. Fortmann-Grote[1], A. P. Mancuso[1,16], T. Kluge[3], C. Gutt[2]

[1]European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany
[2]Universität Siegen, Walter-Flex-Str. 3, 57072 Siegen, Germany
[3]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328, Dresden, Germany
[4]Japan Synchrotron Radiation Research Institute (JASRI), Sayo, Hyogo 679-5198, Japan
[5]RIKEN SPring-8 Center, Sayo, Hyogo 679-5148, Japan
[5]QST-Kansai, KPSI,8-1-7 Umemi-dai, Kizugawa-city, Kyoto, 619-0215, Japan
[7]SLAC National Accelerator Laboratory, Menlo Park, California 94025, USA
[8]Gwangju Institute of Science and Technology (GIST), Gwangju 61005, Republic of Korea
[9]Universität Mainz, Staudinger Weg 7, 55128 Mainz, Germany
[10]Open and Transdisciplinary Research Institute, Osaka University, Suita, Osaka 565-0087, Japan
[11] Graduate School of Engineering, Osaka University, Suita, Osaka 565-0087, Japan
[12]Technische Universität Dortmund, August-Schmidt-Straße 1, 44227, Germany
[13]CEA, DAM, DIF, 91297 Arpajon, France
[14]Helmholtz Institute Jena, Fröbelstieg 3, 07743 Jena, Germany
[15]Institute of Laser Engineering, Osaka University, Suita, Osaka 565-0871, Japan
[16]Department of Chemistry and Physics, La Trobe Institute for Molecular Science, La Trobe University, Melbourne, Victoria 3086, Australia

The interaction of intense laser pulses with solid matter initiates ultrafast surface electron density modulations on the nanometre (nm) scale, which provides a basis for technological developments in areas from material processing, surface nanostructuring to relativistic plasma optics. Currently, a lack of appropriate surface and subsurface methodology to track density dynamics with sufficient spatial and temporal resolution restricts quantitative understanding, and eventual control, of the laser-solid interaction and the subsequent energy transport into the bulk. We recently proposed a novel method for in situ visualization of nanometer depth-resolved density dynamics by grazing-incidence x-ray diffuse scattering with an XFEL. Our first proof-of-principle experiment at SACLA facility showed how the surface ablation and density perturbation following the femtosecond laser pulse interaction with multilayer samples develop over time [1]. This new methodology opens up new possibilities for accurate characterization of surface and subsurface dynamics in various applications including laser ablation, creation of warm-dense-matter, dynamic compression, and relativistic laser-plasmas.

[1] L. Randolph, M. Banjafar, T. R. Preston et al., arXiv preprint 2012.15076

Thursday
23 Sep
12:30

HED science with intense heavy-ion pulses at GSI/FAIR

Paul Neumayer

GSI Helmholtz-Zentrum für Schwerionenforschung GmbH

The facility FAIR, currently under construction at the GSI Helmholtzzentrum für Schwerionenforschung, will deliver short heavy-ion pulses at unprecedented fluences. Within the framework of the HED@FAIR collaboration we are preparing an experimental station where such pulses can be used for volumetric heating of mm-scale samples to electron-volt temperatures, providing a novel path to generating matter at extreme conditions. Comissioning of the infrastructure and early proof-of-principle experiments are currently being carried out at an existing irradiation area at GSI. We will present first results testing ion beam focusing and heating with $> 2 \cdot 10^9$ Xe-ion pulses, as well as diagnostic schemes based on intense x-ray sources driven by GSI's highenergy laser facility PHELIX. This paves the way to first heavy-ion pump - x-ray probe experiments foreseen in 2022.

Thursday
23 Sep
14:30

High Resolution Inelastic X-ray scattering experiments on laser-compressed argon

E.E McBride

SLAC National Accelerator Laboratory, Stanford, USA

For extreme states of matter produced in the laboratory, direct and accurate measurements of thermodynamic and transport properties are vital to guide the development of theoretical models. One technique to create such systems is to couple dynamic laser-driven compression and laser heating techniques to access pressure and temperature similar to those found inside the core of planets. While it is possible to directly investigate the density and pressure of a material under dynamic compression, measuring the temperature of the bulk temperature remains a challenge. Common techniques such as Streaked Optical Pyrometry, rely on a priori knowledge of the matter under investigation and give accurate measurements above 4000 K. In contrast, Inelastic X-ray Scattering at an X-ray Free Electron Laser offers a unique capability to measure the bulk temperature from low energy collective oscillation of the electron density and the principle of detailed balance. Here, I will discuss the method and its validation from measurements taken at the High Energy Density end station at the European XFEL on resistively heated single crystal Diamond. Finally, I will present the application of this method to measure the ion temperature of shock compressed Argon at the Matter in Extreme Condition at the Linac Coherent Light Source.

Characterizing the Ionization Potential Depression in Dense Plasmas with High-Precision Spectrally Resolved X-ray Scattering

Thursday 23 Sep 15:10

Oliver Humphries[1], Julian Lütgert[1], Katja Voigt[1], Michael Stevenson[2], and Dominik Kraus[1,2]

[1] Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

[2] Institute of Physics, University of Rostock, Albert-Einstein-Str. 23, 18057 Rostock, Germany

Details of a recent experiment at the European XFEL will be presented, studying the ultrafast creation of dense plasmas by isochoric heating, and characterizing their properties. The high-precision X-ray scattering diagnostic used is particularly well-suited to probe the ionization potential depression as well as ionization and temperature. This approach has a high potential to resolve existing discrepancies on ionization potential depression models that are important for modelling celestial bodies like giant planets, Brown Dwarfs and stars as well as for several technological applications including intense laser matter interaction and radiation damage research.

X-rays as Drivers of HED Experiments

Thursday 23 Sep 15:30

N. J. Hartley[1,2], P. Heimann[1], D. Kraus[2,3], E. E. McBride[1]

[1] SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA

[2] Helmholtz-Zentrum Dresden-Rossendorf, Dresden 01328, Germany

[3] Institute for Physics, University of Rostock, Rostock 18059, Germany

With short pulse lengths and high sample penetration, intense beams from X-ray Free Electron Lasers offer unique capabilities as drivers of high energy density states. Much of the behavior that they induce is best understood by generating multiple pulses, allowing samples to be both pumped and probed by Xrays. This talk will cover some of the possible approaches to performing such experiments, including with split undulator modes and split-and-delay lines, present recent X-ray pump-probe results from SACLA and LCLS, on a variety of different materials, as well as outline proposed future work at these and other facilities.

Thursday
23 Sep
15:50

Temperature relaxation in strongly-coupled binary ionic mixtures

Luciano G. Silvestri[1],R. T. Sprenkle[2], S. D. Bergeson[2], M. S. Murillo[1]

[1] Michigan State University, East Lansing, MI, 48824, USA
[2] Brigham Young University, Provo, UT 84602, USA

Relaxation in non-ideal plasmas is a complex process that involves expansions or contractions, thermal conduction, thermalization and temperature equilibration. Unfortunately, very little is known experimentally about these processes because of the challenges associated with isolating them individually. As such, we rely heavily on unvalidated theoretical models. This knowledge gap is particularly large for the very challenging case of ionic relaxation. Current improvements in experimental techniques now allow for the creation of ultracold binary mixtures for the investigation of equilibrium relaxation phenomena dominated by ion-ion collisions. These experiments, when complemented by large-scale molecular dynamics (MD) simulations, promise to provide detailed data on these processes. We have modeled a binary relaxing ultracold neutral plasma with MD, motivated by experiments at Brigham Young University, and compared the results to the most common theoretical models. None of the temperature relaxation rates from current theoretical models is within an order of magnitude of the MD simulations, suggesting serious gaps in our knowledge of ionic relaxation. We argue that such disagreement is due to dynamical correlations neglected by the currently available theoretical models.
silves28@msu.edu

Physics beyond homogeneous warm dense matter

Friday
24 Sep
09:00

Zhandos Moldabekov

Center of Advanced Systems Understanding (CASUS), Untermarkt 20, 02826 Görlitz, Germany

Warm dense matter (WDM) is a state of matter covering parameter space between solids and dense plasmas, and is characterized by the simultaneous relevance of electronic quantum degeneracy, thermal excitations, and strong inter-particle correlations. WDM is an interdisciplinary field between plasma physics, condensed matter physics, high pressure science, inertial confinement fusion, planetary science, and materials science under extreme conditions [1-3]. Therefore, WDM is a complex regime to which neither ordinary condensed matter theory nor plasma theory are applicable. In particular, a highly ionized WDM state is closely related to a non-ideal dense plasma state. Parameters of relevant WDM experiments are shown in Fig.1 along with other types of plasma states. Due to relatively well developed theoretical and computational methods for homogeneous states, most of the initial studies were focused on uniform WDM. However, recent introduction of THz lasers [4], the novel seeding technique to reach high intensities [5], and laser pumping of a sample with a pre-designed periodic grating structure [6] allows us to generate inhomogeneous states. Therefore, this talk will be focused on inhomogeneous states. In particular, periodically inhomogeneous WDM is considered. The results will be presented for collective oscillations in such systems. It will be shown that such interesting features like double plasmon and optical mode appear in electronic density excitation spectra. Additionally, the non-linear density response of electrons and applicability of various exchange-correlation functionals such as LDA, GGA, and meta-GGA will be discussed. The analysis of the quality of the KS-DFT approach based on different exchange-correlations functionals is performed by comparing to QMC data. Finally, the quantum fluid theory of inhomogeneous quantum electrons will be presented. The results on the first ab inito study of the many-fermion Bohm field will be shown. The latter has impact going well beyond WDM, since it is key quantity of Bohmenian quantum mechanics.

[1] A. Ng, IEEE International Conference on Plasma Science (Cat. No.02CH37340), 2002, pp. 163-, doi: 10.1109/PLASMA.2002.1030367.
[2] F. Graziani, M. P. Desjarlais, R. Redmer, and S. B. Trickey, Frontiers and Challenges in Warm Dense Matter (Springer, 2014).
[3] V. E. Fortov,Extreme States of Matter (Springer, Heidelberg, 2016).
[4] B.K. Ofori-Okai, et al., J. Inst13, P06014 (2018).
[5] T Kluge, et al., Phys. Rev. X 8, 031068 (2018).

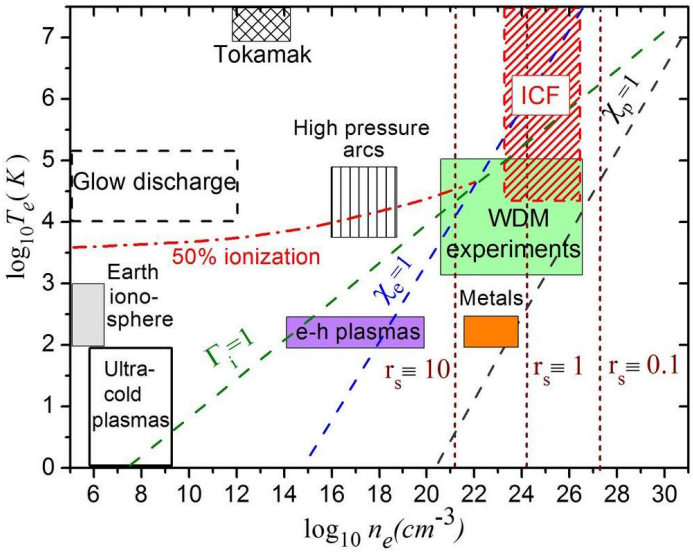

Figure 1: Density-temperature plain with examples of plasmas and characteristic plasma parameters. Figure is from [POP 26, 090601 (2019)].

Friday
24 Sep
09:40

Self-consistent phonon calculations of thermodynamic functions and phase diagram of gold in megabar regime

Xiaoxiang Yu, Bo Chen, Shen Zhang, Dongdong Kang, Jiayu Dai

Department of Physics, National University of Defense Technology, Changsha, 410073, P. R. China

Phase diagram serves as a crucial guideline to determine the structural transformation of materials at extreme conditions, for example shock compression and planet interior. Under the framework of harmonic lattice dynamics, Quasi-harmonic approximation (QHA) method is extensively adopted to calculate the free energy and obtain the phase diagram. However, as confirmed by thermodynamic integration (TI) method, the anharmonicity becomes nonnegligible when temperature goes higher, especially near the phase transition point. Compare with TI method, self-consistent phonon (SCPH) method from anharmonic lattice dynamics possesses the advantages of lower computational cost and ability of decomposing different orders of anharmonicity, is promising for the accurate calculation of the thermodynamic properties and phase diagram. In this work, we used the SCPH theory to include the anharmonic contributions to phonon thermodynamic properties of gold at elevated temperature. The effect of third-order and fourth-order anharmonicity on heat capacity and free energy of fcc and bcc phase are evaluated respectively. The anharmonicity induces the shift of fcc-bcc phase boundary compared with the QHA results.

Corresponding author: X. Yu, xxyu@nudt.edu.cn; J. Dai, jydai@nudt.edu.cn

---

Ionization potential depression in partially ionized plasmas

Friday 24 Sep 10:00

A.E. Davletov, F. Kurbanov, Ye.S. Mukhametkarimov, L.T. Yerimbetova, A.G. Turbekova

Al-Farabi Kazakh National University

In the contemporary physics of warm dense matter, the problem of ionization potential depression is actively discussed. True that if an isolated atom or ion has certain ionization energy, the presence of surrounding plasma particles eventually results in its decrease. This problem was first addressed in the 60's of the last century when two approaches were proposed [1,2] that gave rather contradicting quantitative and qualitative predictions. However, accuracy of experimental techniques of that time was insufficient for making choice between these two concepts, but recent extensive studies of warm dense matter changed the situation dramatically, since they provided a significant increase in sample densities. Direct comparison of theoretical and experimental data turned out to be ambiguous, which necessitates further development of our implication into the subject. Herein we develop a thermodynamical point of view on the problem of the ionization potential depression. Particularly, the self-consistent chemical model of partially ionized plasmas [3] is applied to a system containing electrons, ions and neutral particles. An analytical expression is obtained for the ionization potential depression of neutral particles, which retains its validity for an arbitrary degree of ionization. It is demonstrated that the ionization potential depression is directly related to the interparticle interaction potentials, which can mimic various physical effects. Two limiting cases of low and high ionization degrees are independently considered to show that simple analytical formulas can be neatly derived. It is demonstrated that in case of the hydrogen plasma the results of [4] are restored for the ionization potential lowering of hydrogen atoms.

[1] Stewart J.C., Pyatt K.D. Astrophys. J. 144, 1203 (1966).
[2] Ecker G., Kröll W. Phys. Fluids 6, 62 (1963).
[2] Arkhipov Y., Baimbetov F., Davletov A. Phys. Rev. E 83, 016405 (2011).
[3] Davletov A.E., Kurbanov F., Mukhametkarimov Ye.S. Phys. Rev. E 101, 063203 (2020).

Self-Consistent Relaxation Theory of Collective Dynamics in Coulomb and Yukawa One Component Plasmas

Friday 24 Sep 10:20

Anatolii V. Mokshin and Ilnaz I. Fairushin

Kazan Federal University, Kazan, Russia

One-component strongly coupled plasma is the most suitable many-particle system for the development of the microscopic theory of liquids. This is mainly due to the specific potential of interparticle interaction, as well as a fairly large array of available experimental data and results of molecular dynamics calculations, which can be used to check the correctness of theoretical conclusions [1-3]. In this paper, we will present a microscopic theory of the collective dynamics of particles (ions) of a one-component plasma, where only interaction potentials - the Yukawa and Coulomb

potential - and structural characteristics - the pair distribution function of particles and the structure factor are used as input parameters. The main experimentally measured characteristics of the equilibrium collective dynamics of ions - the spectra of the dynamic structure factor, dispersion laws, the speed of sound, and sound attenuation - are determined within the framework of the theory without using any adjustable parameters. The obtained theoretical results are compared with the results of well-known theoretical models and approaches. This study represents direct realization of the key idea of statistical mechanics that for theoretical description of the collective dynamics of equilibrium fluids, it is sufficient to know the potential of particle interaction and characteristics of the structure.

This work was supported by the Russian Science Foundation (Project No. 19-12-00022).

[1] Z. Donko, G.J. Kalman and P. Hartmann, J. Phys.: Condens. Matter, 21, 413101, 2008.
[2] Yu.V. Arkhipov et al.. Phys. Rev. Lett., 119, 045001, 2017.
[3] A.V. Mokshin and B.N. Galimzyanov, J. Phys.: Condens. Matter, 30, 085102, 2018.

Molecular dynamics simulations of initial stage of hydrocarbon plasma dust nucleation

Friday
24 Sep
11:10

G-C. Otakandza-Kandjani[1], P. Brault[1], M. Mikikian[1], E. von Wahl[1], G. Tétard[2], A. Michau[2], J. Mougenot[2], K. Hassouni[2]

[1] GREMI CNRS -Université d'Orléans, 45067 Orléans Cedex 2, France
[2] LSPM CNRS, Université Sorbonne Paris Nord, 93430 Villetaneuse, France

Complex Non-equilibrium Hydro-Carbon Plasmas (CNHCP) are weakly ionized gases containing electrons, neutral and charged molecular species, large clusters and, possibly, solid particles. They are nowadays a major tool for the elaboration of advanced carbon materials and nanostructures and several key-applications – drugs sensors, electronic devices, optoelectronics, energy storage, flue gas treatment and fuel conversion – are expected to benefit from the precise control of such plasmas. An analogy can be done with the silicon chemistry that has largely benefitted from advanced plasma studies in the past, resulting in outstanding progress in photovoltaics and microelectronics. The HC chemistry leading to large molecular species is also of high interest in astrophysics, planetary atmospheres or circumstellar environments. Despite their large appeal, CNHCP remain very poorly understood because they are governed by phenomena of highly diverse nature and taking place on scales ranging from the molecule to the size of the plasma, i.e., gas phase collisional processes e.g. electronatom/molecule dissociations, excitations and ionizations, (radical) ion collisions, plasma-surface interaction processes, nanoparticle (NP) growth and dynamics, transport phenomena, collective and dusty plasma effects, etc. Thus, CNHCP are often used as black-boxes, limiting their extraordinary potential that cannot be exploited without a real breakthrough in the understanding of the fundamental

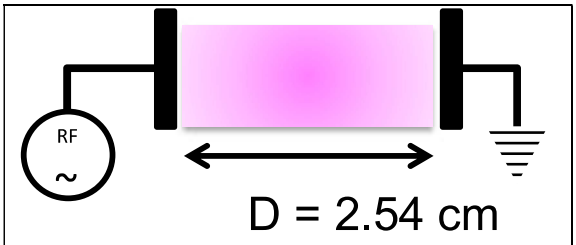

Fig. 1: schematics of the 1D axisymmetric RF plasma. P = 70 Pa, Vb 100 V, T = 300, 400, 500 and 1000K

Table 1: Composition of the 1D plasma model

Major neutral species	molar fractions (Ar is 1.)
H_2	$3.20\ 10^{-2}$
CH_4	$1.40\ 10^{-2}$
C_2H_4	$5.40\ 10^{-3}$
C_2H	$3.20\ 10^{-3}$
C_2H_2	$2.70\ 10^{-3}$
CH_3	$2.30\ 10^{-3}$

Figure 2: (left) Schematics of the 1D axisymmetric RF plasma. P = 70 Pa, V_b 100 V, T = 300, 400, 500 and 1000K. (right) Composition of the 1D plasma model Major neutral molar fractions species (Ar is 1.)

processes driving their physics and chemistry. Among the fundamental processes of interest soot dust growth is of paramount importance. Due to its molecular nature, reactive molecular dynamics simulations are very relevant [1]. Moreover, there exist powerful hydrocarbon interaction forcefields able to describe such phenomena [2]. Among them, the Reactive Empirical Bond Order (REBO) potential is well suited for describing hydrocarbon radical interactions with surfaces. Most of their features are consistent with DFT calculations [2]. Reactivity and nucleation processes of large molecules up to C_20 are described for plasma composition determined by a 1D model (Fig. 2) [3]. Deduced composition is used for building the simulation box. Plasma composition of pure C_2H_2, pure CH_4, CH_4 diluted in Ar (Table 1) are studied and both final composition and nucleation rates are determined.

[1] E. Neyts, P. Brault, Plasma Processes and Polymers 14 (2017) 1600145.
[2] M. Zarshenas et al, J. Phys. Chem. C 122 (2018) 15252-15263.
[3] G. Tetard et al, Plasma Sources Sci. Technol. (2021) submitted.

This work was partly supported by the French National Research Agency (ANR) through the MONA project (ANR-18-CE30-0016)

pascal.brault@univ-orleans.fr

Effective macroions charge in modified Debye-Hückel plus hole and Wigner-Seitz approximations with regard to microions correlations

Friday
24 Sep
11:30

Inna Martynova

Joint Institute for High Temperatures RAS

Features of high-charged macroions screening by microions are analyzed in classical asymmetrically charged complex plasmas when microions correlations are taken into account. We consider a two-component electroneutral system of classical macroions with charges Z ($Z \gg 1$) and oppositely charged microions (i) in a spherically symmetrical electroneutral Wigner–Seitz cell with a central macroion in its center, (ii) in the modified [1] Debye-Hückel plus hole (DHH) approximation [2] with regard to nonlinear screening in the hole. We show that if the microions correlations are taken into account in these two cases (i) and (ii), microions distribution consist of fragments that differ significantly in density and structure. These gaps of the equilibrium microions distribution form the basis of the effective charge definition concept. All microions are subdivided into bound (high-density) layer with total charge Z_b and free (low density) "atmosphere" with charge Z_{fr}. The effective charge is defined as $Z^* \equiv Z - Z_b$. According to [3], the structure and the parameters of the abovementioned gap of the equilibrium distribution have a simple and natural interpretation in the terms of initial macro-level event. This interpretation is a phase transition in a non-ideal one-component macro-plasma of microions. The main point is the relation between the effective macroion charge Z* and an initial one Z with regard to a non-linear screening effect and strong microions correlations. The dependence of the effective macroion charge Z* on its initial charge Z has two modes – of weak and strong screening – when the nonlinear screening effect is taken into account. Characteristics of two different parts of the relation between the effective charge and the initial one are calculated [2,3]. The difference in the dependences Z*(Z) when the microions correlations are taken into account or not is shown. Moreover, if we consider the modified DHH approximation (with regard to the nonlinear screening effect), the radius of the hole decreases significantly when microions correlations are taken into account in comparison with the situation with no regard to these correlations.

[1] I. Martynova, I. Iosilevskiy Contrib. Plasma Phys. 2019. V. 59. P. e201800154.
[2] S.A. Khrapak, A.G. Khrapak, A.V. Ivlev, G.E. Morfill Phys. Rev. E. 2014. V. 89. P. 023102.
[3] I. Iosilevskiy Teplofiz. Vys. Temp. 1985. V. 23. P.807.
[4] I. Martynova, I. Iosilevskiy Contrib. Plasma Phys. 2021. V. 61. P. e202000142.
[5] I. Martynova, I. Iosilevskiy,Contrib. Plasma Phys. 2021.P.e202100007.
http://doi.org/10.1002/ctpp.202100007.

Effective symmetry breaking of interparticle interaction in chain structures of microparticles in a gas discharge plasma

Friday 24 Sep 11:50

E.A. Sametov[1,2], E.A. Lisin[1,2], E.A. Kononov[1,2], K. Arkar[1,2], A.A. Alekseevskaya[1,2], M.M. Vasiliev[1,2], O.F. Petrov[1,2,3], J. Carmona-Reyes[3], T.W. Hyde[3]

[1] Joint Institute for High Temperatures, Russian Academy of Sciences, Moscow, 125412 Russia

[2] Moscow Institute of Physics and Technology (National Research University), Dolgoprudnyi, 141700 Russia

[3] Center for Astrophysics, Space Physics and Engineering Research (CASPER), Baylor University, Waco, TX 76798-7310, USA

A system of micron-sized particles trapped in a plasma with an ionic flow is an example of the so-called "breaking" of the interaction symmetry. Such a formal non-fulfillment of Newton's third law arises when considering a subsystem of particles in a medium, while the medium itself is taken into account indirectly - through the potential of interparticle interaction, dissipative forces, and also as a source of the kinetic energy of particles. It is convenient to study the symmetry breaking of interparticle interaction forces using the example of a two-particle system, since it is not required to consider collective effects. But one of the disadvantages of such systems is that they do not allow us to study the distribution of the wake field that appears behind a dust particle in an anisotropic plasma. One of the solutions to this problem is the use of a multiparticle chain of dust particles. Also, the nonreciprocal type of interaction between dust particles can be the cause of the "anomalous heating" of particles, when microparticles have a higher kinetic energy compared to the temperatures of the neutral, ionic and electronic subsystems. In this case, this manifests itself in an increase (or decrease) in the kinetic temperature of microparticles in the direction of the ion flow and a nonequilibrium distribution of thermal energy between the degrees of freedom. This report presents an experimental study of the nonreciprocal effective interaction between microparticles suspended in RF and DC gas discharges. For this purpose, an experimental method based on an analysis of the spectral density of random processes in an open dissipative system of particles with a chain-like ordering was developed. The proposed method was used to reconstruct the derivatives of the forces of interparticle interaction and the external electric field, as well as the kinetic temperature of stochastic motion of particles and dissipative forces acting both on two interacting particles and on a set of particles with chain-like alignment along an external force field. The experiments in an RF discharge were performed for systems containing from 2 to 8 microparticles suspended in a sheath region at a pressure from 70 to 280 mTorr and a discharge power from 1.6 to 14.3 W. Experiments with two particles levitating in the lower stratum of a DC gas discharge at a pressure of 15 mTorr are analyzed depending on the discharge current (from 0.75 mA to 2.05 mA). It was obtained that in the entire range of discharge parameters, the effective interaction between particles is nonreciprocal. It was shown that the dominant mechanism for heating dust particles in chain structures in gas discharges is the work of effective forces of interparticle interaction.

This work was supported by the Russian Science Foundation (Grant No. 19-12-00354).

Poster Session Monday

Screening and structural properties of dense hydrogen plasmas with partially degenerate semiclassical ions

Monday
20 Sep
17:00

T.N. Ismagambetova[1], R. Redmer[2], T.S. Ramazanov[1], M.T. Gabdulli[1,3]

[1]al-Farabi Kazakh National University, Institute of Experimental and Theoretical Physics (IETP), alFarabi str., 71, Almaty, 050040, KAZAKHSTAN

[2]Institute of Physics, University of Rostock, Albert-Einstein-Straße 23 – 24, Rostock, 18059, GERMANY

[3]Kazakh-British Technical University, Tole bi str., 59, Almaty, 050000, KAZAKHSTAN

In this work we study dense plasmas with ideal or weakly coupled quantum electrons and semiclassical non-ideal ions. The investigation of the interaction between particles in dense plasmas is important in both theory and practical applications, e.g., the physics of giant planets and stars, thermonuclear reactors, and experiments with matter under extreme conditions as carried out at facilities such as NIF [1], magnetized Z-pinch [2,3], and GSI-Darmstadt [4]. At the high densities considered, effects due to the wave nature of the ions are of importance. The ion component was investigated in the framework of a one-component plasma model by incorporating the screening effect due to the surrounding electrons into the effective ion–ion interaction potential [5]. On the basis of the derived ion–ion interaction potential, we calculated the structural properties of semi-classical non-ideal ions using the Ornstein–Zernike equation [6] in the hypernetted chain approximation. We have calculated the ion-ion pair distribution function for a variety of plasma conditions including strong coupling.

[1] O. Hurricane et al., "Fuel gain exceeding unity in an inertially confined fusion implosion", Nature 506, 343 (2014). [2] M. E. Cuneo et al., "Magnetically Driven Implosions for Inertial Confinement Fusion at Sandia National Laboratories", IEEE Trans. Plasma Sci. 40, 3222 (2012).

[3] M. R. Gomez et al., "Experimental Demonstration of Fusion-Relevant Conditions in Magnetized Liner Inertial Fusion", Phys. Rev. Lett. 113, 155003 (2014).

[4] B. Y. Sharkov, D. H. H. Hoffmann, A. A. Golubev, and Y. Zhao, "High energy density physics with intense ion beams", Matter Radiat. Extremes 1, 28 (2016).

[5] T.N. Ismagambetova et al., "Dense plasmas with partially degenerate semiclassical ions: screening and structural properties", Jpn. J. Appl. Phys. 59, SHHA10 (2020).

[6] C. Kittel, "Introduction to Solid State Physics", 8th Int. ed., Wiley, New York (2004).

Study of stimulated Raman forward scattering in presence of azimuthal magnetic field in a density rippled plasma in inertial confinement fusion

Monday
20 Sep
17:00

Oriza Kamboj[a], Ashish Yadav[b], Devki Nandan Gupta[c], John Pasley[d] and Niti Kant[a]

[a]Department of Physics, Lovely Professional University, Punjab, India
[b]Mindfire Solutions, Noida, India
[c]Department of Physics & Astrophysics University of Delhi, Delhi, India
[d]York Plasma Institute, Department of Physics, University of York, United Kingdom

This study observes the growth of stimulated Raman scattering in presence of azimuthal magnetic field and a density rippled plasma in inertial confinement fusion. In the presence of an azimuthal magnetic field, the Gaussian laser beam, propagating through a density rippled plasma, is intensified by forward Raman scattering, resulting in two radially localised electromagnetic sideband waves and a lower hybrid wave. In the presence of density rippled plasma, the nonlocal influence induced by the azimuthal magnetic field reduces the nonlocal contact area and, as a result the growth rate, thereby minimizing the possibility of pre-heating of plasma in ICF.

[1] J. Nuckolls and L.Wood, Nature (London) 239, 139 (1972).
[2] J. Lindl, Phys. Plasmas 2, 3933 (1995).
[3] R. McCrory, J. Soures, C. Verdon, F. Marshall, S. Letzring, S. Skupsky, T. Kessler, R. Kremens, J. Knauer, H. Kim et al., Nature (London) 335, 225 (1988).
[4] W. L. Kruer, The Physics of Laser Plasma Interactions (Westview Press, Boulder, 2003).
[5] W. L. Kruer, The Physics of Laser Plasma Interactions (Addison-Wesley Publishing Company, 1988).
[6] J. D. Moody, P. Datte, K. Krauter, E. Bond, P. A. Michel, S. H. Glenzer, L. Divol, C. Niemann, L. Suter, N. Meezan, B. J. MacGowan, R. Hibbard, R. London, J. Kilkenny, R. Wallace, J. L. Kline, K. Knittel, G. Frieders, B. Golick, G. Ross, K. Widmann, J. Jackson, S. Vernon, and T. Clancy, Rev. Sci. Instrum. 81, 10D921 (2010).
[7] C. Rousseaux, G. Huser, P. Loiseau, M. Casanova, E. Alozy, B. Villette, R. Wrobel, O. Henry, and D. Raffestin, Phys. Plasams 22, 022706 (2015).
[8] Igumenshchev, W. Seka, A. A. Solodov, A. V. Maximov, J. A. Marozas, T. J. B. Collins, D. Turnbull, F. J. Marshall, A. Shvydky, J. P. Knauer, R. L. McCrory, A. B. Sefkow, M. Hohenberger, P. A. Michel, T. Chapman, L. Masse, C. Goyon, S. Ross, J. W. Bates, M. Karasik, J. Oh, J. Weaver, A. J. Schmitt, K. Obenschain, S. P. Obenschain, S. Reyes, and B. Van Wonterghem, Matter Radiat. Extremes 2, 37 (2017).
[9] D. H. Froula, L. Divol, R. A. London, R. L. Berger, T. D€oppner, N. B. Meezan, J. S. Ross, L. J. Suter, C. Sorce, and S. H. Glenzer, Phys. Rev. Lett. 103, 045006 (2009).
[10] A. Le Cain, G. Riazuelo, and J. M. Sajer, Phys. Plasmas 19, 102704 (2012).
[11] B. J. Albright, L. Yin, and B. Afeyan, Phys. Rev. Lett. 113, 045002 (2014).
[12] Z. J. Liu, C. Y. Zheng, L. H. Cao, B. Li, J. Xiang, and L. Hao, Phys. Plasmas 24, 032701 (2017).

[13] T. Gong, J. Zheng, Z. Li, Y. Ding, D. Yang, G. Hu, and B. Zhao, Phys. Plasams 22, 092706 (2015).
[14] M. J. Rosenberg, et al. Phys. Plasams 27.4 (2020).
email: kambojoriza1964@gmail.com

Laser-ion acceleration in the optimized TNSA regime via temporal pulse shaping

Monday
20 Sep
17:00

Marco Garten[1,2], Ilja Göthel[1,2], Thomas Miethlinger[1,2], Brian Edward Marré[1,2], Tim Ziegler[1,2], Thomas Püschel[1], Stefan Bock[1], Karl Zeil[1], Michael Bussmann[1,3], Thomas Cowan[1], Ulrich Schramm[1,2], and Thomas Kluge[1]

[1]Helmholtz-Zentrum Dresden – Rossendorf, Dresden, Germany
[2]Technische Universität Dresden, Dresden, Germany
[3]Center for Advanced Systems Understanding, Görlitz, Germany

Establishing precise control over the beam parameters of laser-accelerated ions from the interaction of ultrashort ultra-high intensity (UHI) laser pulses with ultrathin foils has been the major goal of the last 20 years since the first description of the TNSA process[1,2]. Especially the quest for repeatable, highest maximum energies continues to be challenging as the spatiotemporal coupling of laser-pulse and target parameters down to the femtosecond-nanometer level was found to be decisive for the overall acceleration performance[3,4]. In particular, precise control and metrology of the driving UHI laser pulses are paramount to achieving this goal[5]. We present a multi-parameter-space study, bridging the scales from picosecond preplasma formation over transient, non-equilibrium dynamics of the tens of femtosecond laser duration down to attosecond plasma oscillations performed through 1D– up to 3D particle-incell simulations. By taking into account realistic temporal intensity contrast features of the last picosecond prior and up to the first picosecond after the main pulse peak, we show how temporal pulse shaping optimizes the TNSA process.
[1] Macchi et al. (2013) Ion acceleration by superintense laser-plasma interaction Rev. Mod. Phys. 85 751–93
[2] Daido et al. (2012) Review of laser-driven ion sources and their applications Reports Prog. Phys. 75 056401
[3] Albert et al. (2020) 2020 Roadmap on Plasma Accelerators New J. Phys. 0–31
[4] Zeil et al. (2012) Direct observation of prompt pre-thermal laser ion sheath acceleration Nat. Commun. 3 874
[5] Ziegler et al. (2021) Proton beam quality enhancement by spectral phase control of a PWclass laser system Sci. Rep. 11 7338

Monday
20 Sep
17:00

In situ atomic physics for PIC

B.E Marré

[1]Helmholtz-Zentrum Dresden – Rossendorf, Dresden, Germany
[2]Technische Universität Dresden, Dresden, Germany

Standard modelling techniques for atomic process in PIC simulation are not sufficient for nonthermal relativistic plasmas, since they either neglect excited states, are not self-consistent with 3d plasma simulations or assume quasi-thermal plasma conditions. To remedy this, we are developing a new Particle-In-Cell-algorithm extension to allow us to model atomic states self consistently with the PIC-simulation, in transient plasmas and without assuming temperatures. This extension is based on a reduced atomic state model, which is directly coupled to the existing PIC-simulation and for which the atomic rate equation is solved explicitly in time. This allows us to model excitation and deexcitation of ions in transient plasma conditions, as typically encountered in laser generated plasmas. This new approach to atomic physics modelling will be very useful in plasma emission prediction, plasma condition probing with XFEL and better understanding of isochoric heating processes, since all of these rely on an accurate prediction of atomic state populations inside transient plasmas.

Monday
20 Sep
17:00

Multimodal dusty plasma in DC glow discharge at temperatures below 2 K

R. E. Boltnev[a,b,c], E. A. Kononova[c], F. M. Trukhachev[a], M. M. Vasiliev[a,c], O. F. Petrova[c]

[a]Joint Institute for High Temperatures, Russian Academy of Sciences, Moscow, 125412, Russia
[b]Chernogolovka Branch of the N. N. Semenov Federal Research Center for Chemical Physics, Russian Academy of Sciences, Chernogolovka, Moscow region, 142432, Russia
[c]Moscow Institute of Physics and Technology, Dolgoprudnyi, Moscow region, 141701, Russia

Experimental studies of ultracold multimodal dusty plasma in a positive column of the glow discharge are discussed. A multimodal complex plasma formed by a spheroidal dusty structure consisting of polydisperse CeO_2 particles superimposed with a cloud of nanoclusters and solid helical filaments was observed and studied at the temperatures below 2 K and and pressure ∼4 Pa. Formation of a liquid-like dusty plasma structure occurred after injection of polydisperse cerium oxide particles in the glow discharge cooled with superfluid helium. It was found that the balance of the gravity and electrostatic forces was matched only for the fraction of particles with sizes from 1 to 6 μm while the initial very broad size distribution spanned from 0.1 to ∼100μm. The particle concentration was estimated of order 10^5 cm^{-3}. The coupling parameter ∼10 determined for the dusty plasma structure corresponds very well to its liquid-like type. The electron concentration in the plasma was estimated ∼ 10^8 cm^{-3}. The cloud of nanoparticles (with the sizes less than 80 nm) and non-linear waves within the cloud were observed at temperatures within

1.6 . . . 2 K. The nanocluster concentration was found as high as $10^6 \ldots 10^7$ cm^{-3}. Charging of nanoclusters in plasma produced a stable uprising nanocluster flow ($\sim 10^8$8 cluster/s) driven by external electrostatic field and observable due to laser light scattering on dust acoustic waves developed within the flow. Temporal variations of the nanocluster concentration caused changes of the interparticle distance in the dusty plasma structure composed of CeO_2 particles. Solid helical filaments with the length up to 5 mm, diameter up to 22 μm, total charges $\sim 10^6$e, levitating in the gas discharge were synthesized at the temperatures $\leq$2 K. It was revealed that intense sputtering of the clay insert due to focused beams of low energy electrons and ions produces a total flow $\sim$100 ng/s of sputtered materials at the power released in the discharge less than 0.1 W.

email: boltnev@gmail.com

The work has been carried out under the support of the Russian Science Foundation (Project # 19-12-00354).

First-principles derivation and properties of density-functional average-atom models

Monday
20 Sep
17:00

T.J. Callow[1], E. Kraisler[2], S.B. Hansen[3] and A. Cangi[1]

[1]CASUS, Görlitz, Germany

[2]Fritz Haber Center for Molecular Dynamics and Institute of Chemistry, The Hebrew University of Jerusalem, Israel

[3]Sandia National Laboratories, Albuquerque, USA

Finite-temperature Kohn–Sham density-functional theory (KS-DFT) is a widely-used method in simulations of materials under warm-dense matter (WDM) conditions. However, due its unfavourable scaling with respect to temperature, there is much interest in developing simplified methods which retain as much as possible the accuracy of full KS-DFT calculations at reduced computational costs. Average-atom (AA) models are a well-established example of such an approach. However, there are various types of AA model, and the limits under which specific models can expect to yield accurate results are not always well understood, limiting their predictive capabilities. In this talk, we present a first-principles derivation of a KS-AA model: we reduce the fully-interacting system of electrons and nuclei to a single atom under appropriate boundary conditions, carefully analysing the assumptions made and terms neglected in this derivation. Using this model, we compute some common properties for a range of temperatures and densities: our results highlight the importance of the choice of boundary conditions and the significance of the self-interaction error. We discuss the implications of these findings, and possible strategies to reduce the impact of common errors, for users and developers of AA models.

Application of intense ion beams to planetary physics research at the FAIR facility

Monday 20 Sep 17:00

N.A. Tahir[1], A. Shutov[2], P. Neumayer[1], V. Bagnoud[1], A.R. Piriz[3] and S.A. Piriz[3]

[1]GSI Darmstadt, Germany
[2]IPCP Chernogolovka, Russia
[3]UCLM, Ciudad Real, Spain

Discovery of thousands of extrasolar planets of different type including gas giants, water rich as well as rocky planets has led to a much greater interest in planetary physics research. Existing planetary models predict that extreme physical conditions including ultra-high pressures (5-30 Mbar), super-solid density, but relatively low temperatures (5000-20000 K) exist in the planetary interiors. To have a better understanding of the processes of planetary formation and evolution, it is necessary to study the thermophysical and transport properties of matter under such extreme conditions in the laboratory. Theoretical work has shown that intense heavy ion beams are a very efficient tool to implode material samples to induce planetary core conditions. The heavy ion synchrotron, SIS100, which is under construction at the Facility for Antiprotons and Ion Research [FAIR] at Darmstadt, will deliver strongly bunched, well focused energetic intense ion beams with unprecedented intensities. Numerical simulations have shown that using the FAIR beam parameters, it is possible to generate core conditions of hydrogen rich planets like Jupiter and Saturn [1], rocky planets like Earth and more massive Earth-like extrasolar planets, the Super-Earths [2], as well as water-rich planets like Uranus and Neptune [3]. Based on these simulation results, a dedicated experiment named LAPLAS [Laboratory Planetary Sciences] has been proposed as part of the FAIR High Energy Density program. An overview of this work is given in this presentation.

[1] N.A. Tahir et al, "Metallization of hydrogen using heavy-ion-beam implosion of multi-layered cylindrical targets", Phys. Rev. E 63, 016402 (2001).
[2] N.A. Tahir, "Studies of the core conditions of the Earth and Super-Earths using intense ion beams at FAIR", Astrophysical J. Suppl. Series 232:1, 2017 September.
[3] N.A. Tahir, "Production of warm dense water in the laboratory using intense ion beams at FAIR: Application to planetary physics research", Phys. Plasmas 28, 032712 (2021).

Influence of picosecond range laser temporal pulse shape on TNSA ion acceleration

Monday 20 Sep 17:00

Ilja Göthel[1,2], Marco Garten[1,2] Thomas Miethlinger[1], Brian Edward Marré[1,2], Thomas Püschel[1], Tim Ziegler[1,2], Karl Zeil[1], Michael Bussmann[1,3], Ulrich Schramm[1,2], and Thomas Kluge[1]

[1]Helmholtz-Zentrum Dresden – Rossendorf, Dresden, Germany
[2]Technische Universität Dresden, Germany
[3]Center for Advanced Systems Understanding, Görlitz, Germany

It has been shown in recent experiments on laser driven ion acceleration with thin plastic foils, that controlling the temporal beam profile of the driving laser is of a

high importance for achieving a good acceleration performance and high stability. The application of spectral phase terms of second and third order to an ultra high intensity ultrashort laser pulse allows to control the temporal profile in the sub-picosecond range and thereby reliably increase the proton cutoff energy and reduce fluctuations between shots. Those modifications to the spectral phase change the temporal profile in a complex way on all time scales from sub-FWHM-shaping to influences on the picosecond-scale. We present a broad simulational study of the influence of the features of the temporal profile. The realistic (measured and constructed analytically from phase shift) profile is modelled by features like pre- and postpulses, exponential rising ramp and mainpulse skewness. The influence of those features, mainly in the regime of an enhanced TNSA acceleration mechanism, is studied with the features decoupled from each other and in combination, to shed light on recent experimental results as well as develop a predictive picture of the interaction under realistic laser pulse conditions.

Behavior of Dust Particles in Magnetized DC Glow Discharge

Monday
20 Sep
17:00

A.R. Abdirakhmanov[1], L.G. D'yachkov[2], N.Kh. Bastykova[1], M.K. Dosbolayev[1], S.K. Kodanova[1], T.S. Ramazanov[1]

[1]Institute of Experimental and Theoretical Physics, Al-Farabi Kazakh National University, Almaty, Kazakhstan

[2]Joint Institute for High Temperatures, Russian Academy of Sciences, Moscow, Russia

The effect of an external magnetic field on the behavior of dust particles is one of the most intensive topics of dusty plasma experiments. The properties of dust structures in a weak/strong uniform magnetic field in a glow discharge have been experimentally investigated in previous reports [1-3]. However, currently we have limited information about dust structures in a glow discharge in inhomogeneous magnetic fields [4]. Moreover, the behavior of dust structures in a glow discharge in a transverse magnetic field is an unresolved issue and therefore of great interest. This report presents experimental and theoretical results on the investigation of the dust particles behavior in a weak inhomogeneous magnetic field and in a transverse magnetic field produced by a Helmholtz coil in a stratified DC glow discharge are presented. During the experiments with an inhomogeneous magnetic field, it was observed that in the region above the coil the dust structure rotates in a clockwise direction and in the region below the coil the structure rotates in a counterclockwise direction. It is considered that the rotational motion mechanism is devoted to the collisional interactions with the azimuthal ion flux induced by the radial component of the magnetic field and the axial component of the electric field. In addition, numerical calculations of the velocities and angular velocities of monodisperse dust particles are obtained for various values of the magnetic field strength, which has a good agreement with the experimental data. Another experiment concerning the effect of a transverse magnetic field showed a rotating dust vortex in a stratum in the horizontal plane. The rotational feature of the dust vortices was analyzed using the Particle Image Velocimetry (PIV) method.

[1] V.Yu. Karasev, E.S. Dzlieva, S.I. Pavlov, M.A. Ermolenko, L.A. Novikov, S.A. Maiorov, "The Dynamics of Dust Structures under Magnetic Field in Stratified Glow Discharge, Contributions to Plasma Physics 56, 197-203 (2016).
[2] M.M. Vasiliev, L.G. D'yachkov, S.N. Antipov, R. Huijink, O.F. Petrov, and V.E. Fortov, "Dynamics of dust structures in a dc discharge under action of axial magnetic field", EPL,9315001 (2011)
[3] E.S. Dzlieva, L.G. D'yachkov, L.A. Novikov, S.I. Pavlov and V.Yu. Karasev "Fast rotation of dust particle structures in dc glow discharge in a strong magnetic field", Plasma Sources Sci. Technol. 28, 085020 (2019).
[4] A. R. Abdirakhmanov, Zh. A. Moldabekov, S. K. Kodanova, M. K. Dosbolayev, and T. S. Ramazanov "Rotation of Dust Structures in a Magnetic Field in a DC Glow Discharge, IEEE Transaction on Plasma Science 47, 3036-3040 (2019)
This research has been funded by the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan (Grant No AP08855651).

Monday
20 Sep
17:00

Active motion of Janus particle in RF Plasma

Kyaw Arkar[1], M. M. Vasiliev[1,2], O. F. Petrov[1,2], E.A. Kononov[1,2], F. M. Trukhachev[1,2], R.A. Boltnev[1,2]

[1]Joint Institute for High Temperatures, Russian Academy of Sciences, 125412 Moscow, Russia

[2]Moscow Institute of Physics and Technology, 141701 Dolgoprudny, Russia

Janus particles are special types of micron-sized particles, the surface of which is divided into two or more parts with different physical properties [1,2]. This unique feature of Janus particles gives them special properties. Recently, research on Janus particles has been carried out in the fields of chemistry, biology, physics, etc. Laboratory dusty plasma is a convenient object for studying the properties of such particles [3,4,5]. Our research is devoted to the study of the active motion of Janus particles in an electrostatic trap in RF plasma. Active motion is induced by laser radiation. "Active motion" is the property of microparticles to convert energy of their environment into the energy of directed movement [6]. Particles with these properties are called active Brownian particles. Research on active particles and active mater is of both fundamental and applied importance [5,7,8]. In our paper, we presented the studies of the active motion of Janus micro-particles induced by laser radiation in the RF plasma. The uniqueness of the work li
es in the comparison of the parameters of motion of the same spherical melamineformalehyde (MF) particles with different types of coating under the same conditions. Particle types: homogeneous particles; CU coated particles; Janus particles (MF particles partially coated with iron). Janus particles were fabricated according to [5]. The experiments are carried out in a RF discharge chamber. Argon is used as a buffer gas at a pressure of 3.5 Pa. Plasma is ignited between two flat horizontally oriented electrodes; the parameters of the RF generator are voltage 300 V and frequency 13.56 MHz. A copper ring 35 mm in diameter is placed on the lower electrode in order to form an electrostatic trap [9]. Dust particles are injected into the discharge through a window in the upper electrode [10]. Visualization and kinetic

heating of particles is carried out by homogeneous radiation, which is generated by an argon laser with a wavelength of 514 nm. The parameters of the dust particles motion are recorded by a high-speed video camera (400 fps, 1440×1440 pixels). In the course of the experiments, the motion of single dust particles placed in an electrostatic trap under the influence of radiation of different power is investigated. It is shown that dust particles in RF discharge can transform the energy of the laser radiation into their kinetic energy. The absorption of laser energy by the surface of the particle produces a thermophoretic force that determines the particle activity. We observed the regular or irregular active Brownian motion caused by the action of thermophoretic force for various laser intensities. Various types of particle active motion are detected.

[1] Luoni F., Single Janus Particles in a Complex Plasma Environment. Master's Thesis, Politecnico di Milano, Milan, Italy, 2018.
[2] Perro A., Reculusa S., Ravaine S., Bourgeat-Lamic E., Duguet E. J. Mater. Chem., 15, 3745 (2005).
[3] Chen R. T., Muir B. W., Such G. K., Postma A., McLean K. M., Chemical Communications, 28, 5121-3 (2010).
[4] Nosenko V., Luoni F., Kaouk A., Rubin-Zuzic M., Thomas H., Phys. Rev. Research, 2, 033226 (2020).
[5] Arkar Kyaw, Vasiliev M. M., Petrov O. F., Kononov E. A., Trukhachev F. M., Molecules, 26(3), 561 (2021).
[6] Bechinger C., Di Leonardo, R., Löwen H., Reichhardt C., Volpe G., Rev. Mod. Phys., 88, 045006 (2016).
[7] Zhang J., Luijten E., Grzybowski B.A.; Granick S., Chem. Soc. Rev., 46, 5551 (2017).
[8] Kümmel F., ten Hagen B., Wittkowski R., Buttinoni I., Eichhorn R., Volpe G., Löwen H., Bechinger C., Phys. Rev. Lett., 110, 198302 (2013).
[9] Koss X.G., Petrov O.F., Statsenko K.B., Vasiliev M.M., EPL, 124, 45001 (2018).
[10] Vasiliev M.M., Petrov O.F., Alekseevskaya A.A., Ivanov A.S., Vasilieva E.V., Molecules, 25, 3375 (2020).
The study was supported by the Russian Science Foundation (project No. 20-12-00372).

Investigation of the influence of the neutral shadowing force on the properties of dusty plasma using the 3D Molecular Dynamics method

Monday
20 Sep
17:00

A.M. Temirbek[1], M.M. Muratov[1,2], M.M.Gabdullin[3], T.S. Ramazanov[1]

[1]IETP, al-Farabi Kazakh National University, Kazakhstan, Almaty
[1]NNLOT, al-Farabi Kazakh National University, Kazakhstan, Almaty
[1]Kazakh-British Technical University (KBTU), Kazakhstan, Almaty

This paper considers influence of neutral shadowing force on the structural and dynamical properties of the three - dimensional (3D) dusty plasma system under cryogenic conditions [1]. The radial distribution function (RDF), mean square displacement (MSD) of three-dimensional modified Yukawa system is calculated via

theoretical approaches and Molecular Dynamics method [2]. The parameter of the neutral shadowing force which appears due to temperature gradient between dusty particles and background gas is varied. In case of studying RDF the influence of the neutral shadowing force is significant at cutoff radius rcut=2 and the curve of RDF has a sharp jump. The corresponding peak characterizes the most probable case of finding a high concentration of particles. With increasing the coupling parameter, this deviation due to the neutral shadowing force becomes more significant. In contrast when rcut = 1, neutral shadowing force has no effect. It was also found that at $\Gamma \geq 100$ the neutral shadowing force leads to subdiffusion on time scales of the order of tens or hundreds of dust particle oscillation periods. In addition, the neutral shadowing force strongly prevents the transition from anomalous diffusion to the normal diffusion regime.In the case of the 3-D system of dust particles the neutral shadowing interaction leads to the increase of the sound speed of the dust acoustic wave.

[1] T. S. Ramazanov, Z. Moldabekov, and M. Muratov, Phys. Plasmas, 2017, vol. 24, no. 5, Art. no. 050701.

[2] T. S. Ramazanov, A. Z. Gabdulin, and Z. A. Moldabekov, IEEE Trans. Plasma Sci., 2015, vol. 43, no. 12, pp. 4187–4189.

email: temirbek.asema@gmail.com

Shielding of charged particle interactions in the presence of neutrals

Monday
20 Sep
17:00

L.T. Yerimbetova, A. Kissan, A.E. Davletov

Al-Farabi Kazakh National University

At present, the interest in studying the field screening phenomenon has significantly increased, which is associated with active researches in such fields as warm dense matter [1], colloidal suspensions [2], and quark-gluon plasmas [3]. In such systems, particles of the medium are charged and, due to the long-range nature of the Coulomb interaction, they largely exhibit collective behavior, which manifests itself in the interparticle interactions as the screening phenomenon. In the classical treatment the screening phenomenon of electric fields in a plasma is solely caused by charged particles, i.e. electrons and ions. In contrast, the present consideration focuses on the influence of the neutral component of a plasma medium in the situation when the medium density is so high that the correlation between the charged and neutral components can no longer be ignored. The consideration is based on the renormalization procedure of interparticle interactions [4], which takes into account collective events and leads to the generalized Poisson-Boltzmann equation relating the true microscopic potentials with their effective macroscopic counterparts. In Fourier space, the set of Poisson-Boltzmann equations turns into a set of algebraic equations, whose solution allows one to obtain Fourier transforms of the macroscopic potentials. Then, the inverse Fourier transform restores the macroscopic interaction potentials in the usual configuration space to clearly demonstrate the effect of neutrals on the interaction of charged particles. In this case, the analytical consideration

of the limiting cases of low and high number densities of neutral particles is consistently implemented.
[1] Dornheim T., Groth S., Bonitz M. Phys. Rep. 744, 1 (2018).
[2] Rivas N., Frijters S., Pagonabarraga I., Harting J. J. Chem. Phys. 148 (14), 144101 (2018).
[3] Yao X., Müller B. Erratum: Phys. Rev. C 9, 014908 (2018).
[4] Arkhipov Y., Baimbetov F., Davletov A. Phys. Rev. E 83 (1), 016405 (2011).

Many-body quantum dynamics based on fluctuations

Monday
20 Sep
17:00

E. Schroedter, M. Bonitz, and J.-P. Joost

Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

Many-body quantum dynamics is a hot topic in a broad range of fields, including systems as diverse as cold atoms in optical lattices, correlated condensed matter systems and dense quantum plasmas and warm dense matter. The goal is the computation of the nonlinear response of the system to a time-dependent external excitation and the subsequent relaxation, fully including quantum, spin and correlation effects. The standard approaches include reduced density operators (RDO) and Nonequilibrium Green functions (NEGF) that give rise to a hierarchy of coupled equations of motion for the reduced quantities, such as the BBGKY-hierarchy of RDO or the Martin-Schwinger hierarchy of NEGF, e.g. [1]. Recently a dramatic speedup of the numerical solutions of the quantum dynamics that include dynamical screening and strong coupling could be achieved [2,3]. Here we explore an independent approach to the quantum dynamics that is based on the time evolution of correlation functions of quantum fluctuations. This is motivated by successful concepts in classical plasmas [4] and various phenomenological stochastic concepts in quantum systems, e.g. [5]. Here we present a rigorous derivation of the hierarchy of equations of fluctuations of the NEGF and compare it to the aforementioned approaches [6].
[1] M. Bonitz, "Quantum Kinetic Theory", 2nd ed. Springer 2016
[2] N. Schlünzen, J.-P. Joost, Phys. Rev. Lett. 124, 076601 (2020)
[3] J.-P. Joost, N. Schlünzen, and M. Bonitz, Phys. Rev. B 101, 245101 (2020)
[4] Yu.L. Klimontovich, "Kinetic Theory of Nonideal Gases and Nonideal Plasmas", Pergamon Press 1982
[5] D. Lacroix, S. Hermanns, C. Hinz, and M. Bonitz, Phys. Rev. B 90, 125112 (2014)
[6] E. Schroedter, J.-P. Joost, and M. Bonitz, to be published

---

Monday
20 Sep
17:00

Excitation cross sections of the hydrogen atom in the dense semiclassical plasmas

A.T. Nuraly , E.O. Shalenov and K.N. Dzhumagulova
IETP, al-Farabi Kazakh National University, Almaty, 050040, Kazakhstan
Department of Physics, Nazarbayev University, Nur-Sultan, 010000, Kazakhstan

High temperature non ideal plasma is found in many astrophysical objects and is used in some important technological plasma installations. Determination of the composition of such plasma has always been a crucial problem in the description of thermodynamic, transport, and other plasma properties. The use of the Saha equation in many cases is not the best method for solving this problem, since even local thermodynamic equilibrium is rarely observed in such systems. An alternative, more adequate way is to solve the kinetic equation of the reactions. To solve the kinetic equation, it is necessary to determine the cross sections of ionization, excitation and recombination. In this work, the cross sections for the excitation of the hydrogen atom by the electron impact [1] were determined and investigated based on the effective interaction potential taking into account screening and diffraction effects [2]. Such effects play an important role in dense semiclassical plasmas. To determine the excitation cross sections, we used the Born approximation method and the sBE (scaling binding excitation) method, which is used for correction of the results of the Born method. Figure 1 shows the dependences of the excitation cross sections on the energy of the incident electron at different values of the Debye screening length. The figure shows comparisons with the results of Ref.[1], obtained on the basis of the Debye-Hückel potential by the convergent-close-coupling method. The figure shows that the results are in good agreement. It can also be noted that with a fall in the Debye length the excitation cross sections decrease. Figure 1. [1]

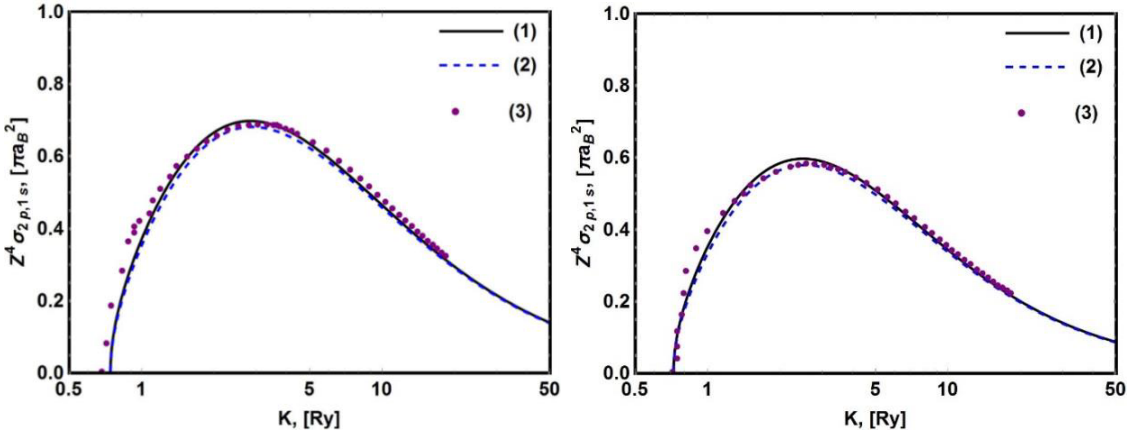

Figure 3: Plots of excitation cross sections $1s \to 2p$: a) $r_D = 20$ a_B; b) $r_D = 10$ a_B. 1 - based on effective potential [2], $\lambda_{ei} = 0$; 2 - based on effective potential [2], $\lambda_{ei} = 0.15$ a_B; 3 - results of work [1].

M. C. Zammit, D. V. Fursa, and I. Bray, Phys. Rev. A 82 (2010) 052705.
[1] T. S. Ramazanov, K. N. Dzhumagulova, Phys. Plasmas 9 (2002) 3758. *e-mail: Shalenov.erik@physics.kz*

Dynamic structure factor of correlated magnetized plasmas

Monday 20 Sep 17:00

Hanno Kählert

Christian-Albrechts-Universität zu Kiel, Germany

Magnetized plasmas display a rich spectrum of collective modes. In this contribution, waves in the magnetized one-component plasma are analyzed by computing the dynamic structure factor with molecular dynamics simulations. Of special interest is the transition from the weakly to the strongly coupled regime. In both limits, a variety of different wave modes are known to exist, including the famous Bernstein modes in weakly coupled plasmas [1] or a set of hybrid modes in the strongly coupled domain [2]. The simulations allow one to investigate the wave spectrum in different magnetization and coupling regimes and to trace the changes when regime boundaries are crossed. The results are compared with analytical approaches to the mode spectrum.

[1] I. B. Bernstein, Phys. Rev. 109, 10 (1958).
[2] T. Ott, H. Kählert, A. Reynolds, and M. Bonitz, Phys. Rev. Lett. 108, 255002 (2012).

Optical properties of binary ionic mixtures

Monday 20 Sep 17:00

Yu.V. Arkhipov[1], A.B. Ashikbayeva[1], A. Askaruly[1], A.E. Davletov[1], I.M. Tkachenko[2]

[1]Al-Farabi Kazakh National University
[2]Universitat Politècnica de València, Spain

Static and dynamic properties of binary ionic mixtures in a thermal equilibrium consisting of two ion species with different ion masses, number densities and positive charge numbers. From the point of view of statistics, the system is classical and there is a negative neutralizing background. The static structure factors of the species are determined in the hyper-netted chain approximation without employing the bridge functions. The system dynamic structure factor and the dispersion and damping of the collective modes are calculated using the self-consistent version of the method of moments [1,2], which permits to express the dynamic characteristics in terms of the static ones (the static structure factor) only without any adjustment to the simulation data and taking the energy dissipation processes into account. The results are compared to the molecular-dynamics data of [3] with satisfactory results. Due to a strong numerical dependence of the dynamic output on the static input, the static data were modified slightly to achieve a numerical agreement between theoretical and simulation results. Further developments are discussed.

[1] Yu. V. Arkhipov et al., Phys. Rev. Lett., 119 (2017) 045001.
[2] Yu. V. Arkhipov et al., Phys. Rev. E 102 (2020) 053215.
[3] J.P. Hansen, I.R. McDonald, P. Vieillefosse, Phys. Rev. A 20 (1979) 2590.

Monday
20 Sep
17:00

Waves in the medium of collisional and viscous quark-gluon plasma

Baiseitov K.

Al-Farabi KazNU, Institute of Experimental and Theoretical Physics, Institute of Applied Science and Information Technology

The focus of this topic is mainly interested in the collective effects of new state of matter called quark-gluon plasma [1,2]. It consists of asymptotically quasi-free quarks and gluons in deconfined state. Such a dense matter was assumed to exist in the core of neutron star in 1960, even before the common accepted theory of strong interaction Quantum Chromodynamics was formulated. Nowadays, we realize that such high densities can occur when quarks focused in small region of space such that they become asymptotically free. QCD has its own problems of divergence in some region of experiments, and this work can be called phenomenological since it does not follow ab initio calculations. In this way, we want to get qualitative understanding of collective effects in quark-gluon plasma. However, in order to study the new state of matter, controlled parameters in experiment is required. These densities and temperature can be reached in experiments on ultra-relativistic heavy-ion collision, e.g. SPS CERN and RHIC BNL experiments operating now, and FAIR SIS and JINR NICA are planned to study the properties quark-gluon plasma. With this amount of experiments conducted especially for the study, direct signatures of quark-gluon plasma formation are not possible to obtain yet, all the signals of quarkgluon plasma formation obtained from particles that leave the matter with it being decayed. Since we have new state of matter, people proposed to study its collective effects, particularly propagation of waves. When we do not have possibility to observe it directly, getting more information about properties of the system gives understanding of quark-gluon plasma formation. For relevant paper about wave properties one can read the following papers. [3, 4] The dispersion relation of waves in medium will be calculated within the frame of two different models that describe quark-gluon plasma. The first is collisional model that is presented by BhatnagarGross-Krook collision operator [5], and the second is viscous model that is derived from hydrodynamic description of quark-gluon plasma [5]. The former can be used to describe weakly coupling system, while the latter shows the properties of more strongly coupled system. In addition, as special case of strongly coupled system, model derived from AdS/CFT duality is used for more complete picture of phenomenon. In this work, it is considered as the special case of viscous quark-gluon plasma, since by adjusting parameters we can reproduce the results obtained from AdS/CFT duality. These two models are taken into account by their dielectric functions that has been calculated in the papers above, and here dispersion relation is presented in the long wavelength limit and in the numerical calculations. Also, phase velocity was calculated in order to compare both models.

[1] Collins, J.C.; Perry, M.J. Superdense Matter: Neutrons or Asymptotically Free Quarks? Phys. Rev. Lett. 1975, 34, 1353.

[2] Cabibbo, N.; Parisi, G. Exponential hadronic spectrum and quark liberation. Phys. Lett. B 1975, 59, 67–69.

[3] K. Baiseitov, Zh.A. Moldabekov, D. Blaschke, N. Djienbekov, and T.S. Ramazanov, Surface waves in collisional quark-gluon plasma. Phys. of part. and nucl.

letters, 17, 6 (2020).
[4] D. A. Fogaça, L. G. Ferreira Filho, and F. S. Navarra, Nonlinear waves in a quark gluon plasma, Phys. Rev. C 81, 055211, 2010
[5] M. E. Carrington, T. Fugleberg, D. Pickering, and M. H. Thoma. Dielectric functions and dispersion relations of ultrarelativistic plasmas with collisions // Can. J. Phys. 82, 671 (2004).
[6] Bing-feng Jiang and Jia-rong Li. The dielectric function of the viscous quark-gluon plasma // Nucl. Phys. A 847, 2010.

Sarkas: A Fast Pure-Python Molecular Dynamics Suite for Non-Ideal Plasmas

Monday
20 Sep
17:00

Luciano G. Silvestri[1], Luke J. Stanek[1], Yongjun Choi[1], and Michael S. Murillo[1], Gautham Dharuman[2]

[1]Michigan State University, East Lansing, MI, 48824, USA
[2]Lawrence Livermore National Laboratory, Livermore, CA, 94550, USA

Molecular Dynamics (MD) is a powerful tool for simulating complex dynamical systems. MD is used across several disciplines and their sub-fields, e.g. biology, chemistry, material science. As a matter of fact for each of these research fields we can find MD codes, open-source or proprietary, optimized for the simulation of their respective dynamical systems. No such code exists for Non-Ideal Plasmas. This generates several difficulties for researchers. On one hand researchers are forced to modify existing codes and/or write their own. This requires an extensive knowledge of computing as all of the available codes have been developed in low-level languages, e.g. C or Fortran. Furthermore, the codes have been optimized for the simulation of systems other than non-ideal plasmas and as such are often difficult to modify. On the other hand most MD codes provide only a code for the simulation phase and lack pre-processing and/or post-processing analysis tools. Several open-source packages are available for post-processing, but again they are specific to systems other than non-ideal plasmas and are often developed in interpretative languages, e.g. Python. Here we present Sarkas: a fast pure-python MD suite for Non-Ideal Plasmas. Sarkas aims at lowering the entry barrier for computational plasma physics by providing a comprehensive MD suite complete of pre- and post-processing tools most common in plasma physics. It offers the ease of use of Python while being highly performant with execution speeds comparable to that of compiled languages. Its high-performance originates from the extensive use of NumPy arrays and Numba's just-in-time compilation. Sarkas is built in a modular fashion to allow easy implementation of additional features. It offers a variety of interaction potentials commonly used in plasma physics, Coulomb, Yukawa, Quantum Statistical Potentials. It is the only MD code to support electrons as dynamical particles. Furthermore, Sarkas' built-in pre-processing and post-processing libraries for data analysis allow researchers to get publication-grade results in less time.
email: silves28@msu.edu

Ab initio path integral Monte Carlo approach to the momentum distribution of the uniform electron gas at finite temperature without fixed nodes

Monday
20 Sep
17:00

Maximilian Böhme

CASUS, Görlitz, Germany

We present extensive new ab intio path integral Monte Carlo results for the momentum distribution function n(k) of the uniform electron gas (UEG) in the warm dense matter (WDM) regime over a broad range of densities and temperatures. This allows us to study the nontrivial exchange–correlation induced increase of low-momentum states around the Fermi temperature, and to investigate its connection to the related lowering of the kinetic energy compared to the ideal Fermi gas. In addition, we investigate the impact of quantum statistics on both n(k) and the off-diagonal density matrix in coordinate space, and find that it cannot be neglected even in the strongly coupled electron liquid regime. Our results were derived without any nodal constraints, and thus constitute a benchmark for other methods and approximations.

Quantum degenerate electron-ion plasmas in the Born-Mermin approximation

Monday
20 Sep
17:00

Paul Hamann[1], Jan Vorberger[2], Tobias Dornheim[3], Michael Bonitz[1]

[1] Christian-Albrechts Universtität Kiel, Kiel, Germany
[2] Helmholtz-Zentrum Dresden-Rossendorf, Dresdne, Germany
[3] CASUS, Görlitz, Germany

Warm dense matter (WDM) is challenging to describe theoretically. Based on recent ab initio PIMC results for the local field correction of the uniform electron gas1 , which provides an accurate description of correlations in the electronic component itself23 , we calculate dynamical properties of quantum degenerate electron-ion plasmas in the Born-Mermin approximation. Moreover we present accurate data for the plasmon dispersion for which we perform an analytical continuation of the dielectric function4 which allows to extend the analysis to strong correlations and strong plasmon damping.

[1] T. Dornheim et al., J. Chem. Phys. 151, 194104 (2019)
[2] T. Dornheim et al., Phys. Rev. Lett. (2018)
[3] P. Hamann et al., Phys. Rev. B (2020)
[4] P. Hamann et al., Contrib. Plasma Phys. (2020)

Thermodynamic properties of the finite–temperature electron gas by the fermionic path integral Monte Carlo method

Monday
20 Sep
17:00

V.S. Filinov,[1] P.R. Levashov[1,2] , and A.S. Larkin[1]

[1] Joint Institute for High Temperatures, Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

[2] Moscow Institute of Physics and Technology, 9 Institutskiy per., Dolgoprudny, Moscow Region, 141700, Russia

The new ab initio quantum path integral Monte Carlo approach has been developed and applied for the entropy difference calculations for the strongly coupled degenerated uniform electron gas (UEG), a well–known model of simple metals. Calculations have been carried out at finite temperature in canonical ensemble over the wide density and temperature ranges. Obtained data may be crucial for density functional theory. Improvements of the developed approach include the Coulomb and exchange interaction of fermions in the basic Monte Carlo cell and its periodic images and the proper change of variables in the path integral measure. The developed approach shows good agreement with available results for fermions even at temperature four times less than the Fermi energy and practically doesn't suffer from the "fermionic sign problem", which takes place in standard path integral Monte Carlo simulations of degenerate fermionic systems. Presented results include pair distribution functions, isochors and isotherms of pressure, internal energy and entropy change in strongly coupled and degenerate UEG in a wide range of density and temperature.

The theoretical development of the UEG model was supported by the Russian Science Foundation, Grant No. 20-42-04421. The path integral Monte Carlo method, its algorithmic realization and extensive numerical calculations of the pair distribution functions, the isochores and isotherms of pressure and internal energy and the entropy changes in the strongly coupled and degenerate UEG in a wide range of density and temperature have been carried out in the frame of the State assignment No. 075-00892-20-01.

Simulation of warm dense deuterium by WPMD-DFT

Monday
20 Sep
17:00

Ya. S. Lavrinenko[1,2], I.V. Morozov[1,2], I.A. Valuev[1]

[1]Joint Institute for High Temperatures of the Russian Academy of Sciences

[2]Moscow Institute of Physics and Technology

The WPMD-DFT simulation method developed recently [1,2] is applied to study the shockcompressed deuterium. The method is based on the wave packet molecular dynamics (WPMD) and density functional theory (DFT). It allows to consider equilibrium and non-equilibrium nonideal plasmas and warm dense matter including simulations of non-adiabatic dynamics of electrons and ions, electron-ion relaxation, etc. In the WPMD-DFT approach, electrons are represented as Gaussian wave packets whereas the Hartree approximation for the many-body wave function is used.

The electron exchange-correlation term is obtained via the local electron density following the DFT approach where the electron density is calculated from wave packet positions and widths. In this work, we report on the method accuracy when calculating the isentrope of the shockcompressed deuterium as well as the Hugoniout adiabat. The isentrope is obtained by both the direct simulation of the plasma compression and by calculation of the equilibrium values of pressure and energy followed by the solution of Zeldovich's equation. The WPMD-DFT simulation results are compared with available experimental data and other simulation approaches. Moreover, the ability to study non-adiabatic processes is demonstrated by simulations of the electron-ion relaxation.

[1] Y. S. Lavrinenko, I. V. Morozov, and I. A. Valuev, Contrib. Plasma Phys. 59, e201800179 (2019).

[2] Lavrinenko Ya.S., Morozov I.V., Valuev I.A., J. Phys. Conf. Ser. 1787, 012043 (2021).

Monday
20 Sep
17:00

Development of a microsecond pulse Joule heating facility for investigating warm dense metallic plasmas

B. Jodar[1,2], A. Marizy[1], E. Lescoute[1,2] and G. De Lachèze-Murel[1,2]

[1]CEA, DAM, DIF, F-91297.

[2]Université Paris-Saclay, CEA, LMCE, 91680 Bruyères-le-Châtel, France

Over the past decades, notable efforts have been devoted to study the thermodynamic and transport properties of metals in the warm dense matter regime. Isochore measurements were performed on the Enceinte à Plasma Isochore facility (EPI), giving access to electrical conductivity and internal energy of homogeneous plasmas up to 1-2 GPa for density ratios comprised between 1/30 and 1/10 of the standard density [1-5]. Experimental data collected with the EPI enabled the validation of theoritical properties of various metals determined from quantum molecular dynamics simulations [6-8]. To explore further the properties of plasmas at higher pressure ($2 \leq p \leq 7$ GPa) and density states ($1/8 \leq \rho/\rho_0 \leq 1/2$), the Enceinte à Plasma Pulsé (EPP) facility has been developed at CEA DAM. The EPP is based on the pulse Joule heating technique [9,10], where micrometer thin metallic foils confined between two saphir plates are heated by a microsecond electrical discharge. In-situ measurements provide access to electrical conductivity and thermodynamics properties such as dissipated internal energy variation, pressure and density. In this presentation will be presented the experimental setup of the EPP facility, implemented in-situ diagnostics and preliminary experiments conducted on aluminium foils.

[1] J. Clérouin, P. Renaudin, Y. Laudernet, and P. Noiret. Electrical conductivity and equationof-state study of warm dense copper : Measurements and quantum molecular dynamics calculations. Physical Review B, 71(064203), 2005.

[2] J. Clérouin, C. Starrett, P. Noiret, P. Renaudin, C. Blancard, and G. Faussurier. Pressure and electrical resistivity measurements on hot expanded metals : Comparisons with quantum molecular dynamics simulations and average-atom approaches. Contribution to Plasma Physics, 52(1) :17–22, 2012.

[3] J. Clérouin, P. Noiret, P. Blottiau, V. Recoules, B. Siberchicot, P. Renaudin, C. Blancard, G. Faussurier, B. Holst, and C.E. Starrett. A database for equations of state and resistivities measurements in the warm dense matter regime. Physics of Plasmas, 19(082702), 2012.
[4] P. Renaudin, C. Blancard, G Faussurier, and P. Noiret. Combined pressure and electricalresistivity measurements of warm dense aluminium and titanium plasmas. Physical Review Letters, 88(21), 2002.
[5] P. Renaudin, C. Blancard, J. Clérouin, G Faussurier, P. Noiret, and V. Recoules. Aluminium equation-of-state data in the warm dense matter regime. Physical Review Letters, 91(7), 2003.
[6] V. Recoules, P. Renaudin, J. Clérouin, P. Noiret, and G. Zérah. Electrical conductivity of hot expanded aluminium : Experimental measurements and ab initio calculations. Physical Review E, 66(056412), 2002.
[7] V. Recoules, J. Clérouin, P. Renaudin, P. Noiret, and G. Zérah. Electrical conductivity of strongly correlated aluminium plasma. Journal of Physics A : Mathematical and General, 36 :6033–6039, 2003.
[8] J. Clérouin, P. Renaudin, V. Recoules, P. Noiret, and M. Desjarlais. Equation of state and electrical conductivity of strongly correlated aluminium and copper plasmas. Contribution to Plasma Physics, 473 :269–272, 2003.
[9] V.N. Korobenko, A.D. Rahkel, A.I. Savvatimskiy, and Fortov V.E. Measurement of the electrical resistivity of hot aluminum passing from the liquid to gaseous state at supercritical pressure. Physical Review B, 71(014208), 2005.
[10] V.N. Korobenko and A.D. Rahkel. Electrical resistivity and equation of state measurements on hot expanded aluminum in the metal-nonmetal transition range. Physical Review B, 75(064208), 2007.

Characterising Insulator-metal transition of Hydrogen with spectrally resolved X-ray scattering

Monday
20 Sep
17:00

D. Ranjan[1,2] , K. Ramakrishna[2] , K. Voigt[2] , O. Humphries[2] , J. Vorberger[2] , and D. Kraus[1,2]

[1]Universität Rostock, Rostock, Germany
[2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The giant planets have dominated the numbers in the ever-increasing list of exoplanets. Efforts to understand the internal structures of these giants have been going on for a few decades. There have been numerous experimental and theoretical endeavours, but there is still a long way to go for a proper understanding of the interiors. The insulator-metal transition in hydrogen is an important phenomenon to understand interiors of gas giants like Jupiter and Saturn and the physical and chemical behavior of highly compressed condensed matter [1]. We discuss potential approach to characterise the formation of metallic hydrogen in dynamically compressed plastic samples by spectrally resolved X-ray scattering. With the help of time-dependent density functional theory (TDDFT) calculations [2] and data previously collected at European X-ray Free-Electron Laser (EuXFEL), wegive an outlook of future experiments, and canvass the possibilities with the drive laser system at EuXFEL.

[1] Jiang, S., Holtgrewe, N., Geballe, Z. M., Lobanov, S. S., Mahmood, M. F., McWilliams, R. S., Goncharov, A. F., A Spectroscopic Study of the Insulator–Metal Transition in Liquid Hydrogen and Deuterium. Adv. Sci. 2020, 7, 1901668.
[2] Kushal Ramakrishna and Jan Vorberger 2020 J. Phys.: Condens. Matter 32 095401.
email: divyanshu.ranjan@uni-rostock.de

Poster Session Thursday

Creation of artificial radiography images to investigate radiation transport in the interior of red dwarfs

Thursday
23 Sep
17:00

Julian Lütgert[1,2] , Mandy Bethkenhagen[3] , Laurent Divol[4] , Tilo Döppner[4] , Gareth N. Hall[4] , Otto L. Landen[4] , Laurent Masse[4,5] , Markus Schörner[4] , and Dominik Kraus[6,1]

[1]HelmholtzZentrum DresdenRossendorf
[2]Technische Universität Dresden
[3]Ecole normale supèrieure de Lyon
[4]Lawrence Livermore National Laboratory
[5]Commissariat á l'énergie atomique et aux énergies alternatives
[6]Universität Rostock, Rostock, Germany

Red dwarfs (M class stars) are the most abundant stars in our solar neighborhood. While convection is believed to be the predominant energy transport mechanism wit hin those objects, the opacity – mainly caused by freefree transitions – determines the efficiency of radiation transfer and is therefore a crucial parameter for modelling red dwarfs. Predictions of freefree absorption (or "inverse Bremsstrahlung") in a regime relevant for the interiors of small stars differ by up to an order of magnitude between different models. An experiment to measure the inquired quantity for the first time, uti lizing the capabilities of the National Ignition Facility to compress hydrogen to ∼800 times ambient densities while preserving moderate temperatures of several 100 eV is currently developed in a campaign within NIF's discovery science program. In this pos ter we present simulated radiography images inferring on the sensitivity of the planned setup and providing impulses for the analysis of the data that will be aquired in 4 shots within the next year.

Thursday
23 Sep
17:00

Characterization of low-density rear-driven collisional plasma jets from thin foils

P. Perez-Martin[1,2], M. Šmíd[1], F. Brack[1,2], P. Cagas[3], M. Červenák[4], P. Gajdos[4], Z. He[5], M. Holec[6], L. Hronová[7], G. Kagan[8], ,N. Kang[5], K. F. Kaniz[9], M. Kozlová[4], F. Kroll[1], X. Pan[1,2], I. Prencipe[1], G. Schaumann[10], S. Singh[4], M. Sobiella[1], B. Srinivasan[3], F. Suzuki-Vidal[11], M. Krus[4], L. Ren[5], K. Falk[1,11]

[1]Helmhotz-Zentrum Dresden-Rossendorf
[2]Technische Universität Dresden
[3]Virignia Tech,
[4]Prague Asterix Laser System
[5]Imperial College London
[6]Lawrence Livermore National Laboratory
[7]Faculty of Nuclear Sciences and Physical Engineering of the Czech Technical University
[8]Imperial College London
[9]Queen's University Belfast
[10]Technische Universität Darmstadt
[11]Czech Academy of Sciences

Collisional, low-density plasma jets are an interesting subject, not only because of their presence in numerous astrophysical phenomena, but also because of their potential as a means to study transport properties in astrophysically relevant plasma, for example, nonlocal electron transport. Despite this, no systematic study that benchmarks the thermodynamic conditions of this kind of jets has been conducted yet. We have carried out two experiments, at the PALS facility at Prague and the SG-II Laser in Shanghai, aimed to characterize plasma jets from thin foils of different thickness and materials. The jets were driven from the rear side of the targets by a kJ class laser. In Prague, we studied jets propagating freely in vacuum, colliding with an obstacle and propagating inside an external magnetic field of varying intensity (5-10 T) and orientation, while at SG-II we explored the scenario of colliding counter propagating jets. Employing a streak camera and a four-frame interferometry setup, we are capable to obtain the velocity and density for an assortment of jets under different conditions and at different stages of development. The density in the colliding jet scenario was measured using x-ray radiography. The free propagation scenario provides insight into the general characteristics of the jet, so that later setups can be specifically tailored around the specific characteristics of the studied foil. The external magnetic field is generated using a pair of pulsed Helmholtz coils, and it reaches intensities of up to 10 T. The evolution of the jet on this conditions is not only interesting on itself, but also an important proof of concept for future plasma transport experiments. The collision with a static object should allow us to generate a compression wave, which translates into a sharp increase of density in the collision area, a feature also present in the colliding jet scenario.

First results from the Ge and quartz x-ray spectrometers at Draco PW laser facility

Thursday 23 Sep 17:00

Radka Štefaníková[1,2] , Xiayun Pan[1,2] , Michal Šmíd[1], Hans-Peter Schlenvoigt[1] , Irene Prencipe[1], Lennart Gaus[1,2], Marvin Elias Paul Umlandt[1,2], Marvin Reimold[1,2] , Tim Ziegler[1], Florian Kroll[1] , Thomas Püschel[1] , Stephan Kraft[1], Ulrich Schramm[1,2], Karl Zeil[1], Josefine Metzkes-Ng[1], Katerina Falk[1,2]

[1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany
[2]Technische Universität Dresden, Dresden, Germany

A large amount of complex processes within laser-produced plasmas put a huge demand for precise diagnostics methods. For example, x-ray emission spectroscopy can be used to study atomic physics and plasma conditions. Here, we introduce two new x-ray spectrometers installed in the Ion acceleration lab at the Draco PW laser facility. Availability of such diagnostics at the Draco PW Ti:sapphire 30 fs laser system (i.e. ultrashort pulse system) allows not only for studying unique plasma conditions driving the ion acceleration, but also exploring new possibilities for x-ray backlighters suitable for high energy density experiments. Both spectrometers are utilized for acquisition of Ti spectral lines, but offer different spectral resolution and range. Quartz crystal spectrometer has wider spectral range, including Ti K-α and He-α emission lines in the spectrum, whereas Ge crystal spectrometer focuses on K-α emission lines and offers 1D spatial imaging. We present first results demonstrating the capabilities of both spectrometers. The first spectroscopic measurements include the emission spectra measurements from flat Ti targets used for proton acceleration calibration and optimization with and without laser pre-pulse and the use of structured targets for enhanced x-ray emission as well as tailoring of the electron spectra for optimization of the proton acceleration process.
email: r.stefanikova@hzdr.de

Investigation of hot dense plasmas heated by short-pulse intense laser using x-ray spectroscopy

Thursday 23 Sep 17:00

Xiayun Pan[1,2], Steffen Sander[3], Michal Šmid[1], Erik Brambrink[4], Vincent Bagnoud[5], James Colgan[6], Tina Ebert[3], Johannes Hornung[5], Daniel Hartnagel[3], Markus Hesse[3], Thomas Kluge[1], Annika Kleinschmidt[5], Pablo Perez-Martin[1,2], Amanda Neukirch[6], Katrin Philipp[2], Gabriel Schaumann[3], Alexandra Tebartz[3], Bernhard Zielbauer[5], Markus Roth[3], Katerina Falk[1,2,7]

[1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany
[2]Technische Universität Dresden, Dresden, Germany
[3]Technische Universität Darmstadt, Darmstadt, Germany
[4]Deutsches Elektronen-Synchrotron, Hamburg, Germany
[5]GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany
[6]Los Alamos National Laboratory, New Mexico, USA
[7]Institute of Physics of the ASCR, Prague, Czech Republic

Hot dense conditions in titanium (Ti) targets irradiated with intense sub-picosecond laser pulses on PHELIX laser facility are investigated using x-ray spectroscopy. The

effects of microstructured targets on laser absorption and conversion efficiency are studied through the K-α emission. The results are benchmarked by flat titanium foils. Two highly oriented pyrolytic graphite (HOPG) crystal spectrometers are utilized to observe the K-α emission from both front and rear sides of Ti targets. The effective temperature and density of hot dense plasmas are evaluated by analyzing the x-ray spectroscopic data in combination with spectral modelling by SCFLY [1], FLYCHK [2] and ATOMIC [3] codes. Particle-in-cell (PIC) simulations are also implemented to study the evolutionary process of the laser-target interaction, providing timedependent electron density and electron energy distribution information, which are used as the inputs of the spectral simulation.

[1] H.-K. Chung et al., High Energy Density Physics 3, 57 (2007)
[2] H.-K. Chung et al., High Energy Density Physics 1, 3 (2005)
[3] P. Hakel et al., Journal of Quantitative Spectroscopy & Radiative Transfer 99, 265 (2006)

E-mail: k.falk@hzdr.de

EXPERIMENTALLY STUDY DAMAGE MECHANISM OF TUNGSTEN MATERIALS USING PLASMA FOCUS DEVICE

Thursday
23 Sep
17:00

Zh.M. Moldabekov, A.M. Zhukeshov, A.T. Gabdullina, A.U. Amrenova
al-Farabi Kazakh National University, Almaty, Kazakhstan

One of the most important tasks of plasma physics [1] is to study the resistance of materials of the first wall, the divertor and other nodes of the thermonuclear reactor to stationary plasma-thermal effects with a capacity of up to 20 mW/m2 and intense pulsed duration of 0.1–10 ms and a power of 1–10 GW/m2 [1–3]. Many of the basic problems investigated and solved but one of the main problems still not enough investigated is connected with material science and radiation nuclear physics [1–5]. They are long lasting irradiation and heat loads that are generated in the fusion devices affect the construction materials and appearance different of defects on the surface materials. In this report presents tungsten materials were studied when it was exposed with deuterium plasma. The experiment was carried out on a plasma focus device with energy of 1.9 kJ, with a pressure of 2.5 torr of deuterium. Some analysis showes formation of different types of damage to the surface of materials when irradiated with pulsed plasma flows of high power and shows that this can cause deep erosion of the material. AFM analysis indicated that cracks up to 2 microns and holes from 81 to 281 nm are found on steel surfaces.

[1] S.H. Saw, V. Damideh, Jalil Ali, R.S. Rawat, P. Lee , S. Lee Damage Study of Irradiated Tungsten using fast focus mode of a 2.2 kJ plasma focus . Vacuum 144 (2017) 14e20.
[2] S. Lee, S.H. Saw, Plasma focus ion beam fluence and flux for various gases, Phys. Plasmas 20 (062702) (2013).
[3] Baluc, N., Schäublin, R., Spätig, P., Victoria, M. On the potentiality of using ferritic/martensitic steels as structural materials for fusion reactors. Nucl. Fusion, 2004, Vol. 44, P. 56–61.

[4] O.V Ogorodnikova. Fundamental aspects of deuterium retention in tungsten at high flux plasma exposure. Journal of Applied Physics, 118:074902, 2015. doi: 10.1063/1.4928407. URL http://dx.doi.org/10.1063/1.4928407.
[5] Xiaolong Jiang, Ying Liu, Bilali Muhutijiang, Zhengkun Liu, Keqiang Qiu, Xiangdong Xu, Yilin Hong, Shaojun Fu, Investigation on morphology and evolution process of plasma induced pitting damage during the ICP etching of fused silica, Vacuum 12 (2016) 121e125.

Recovery Methods for Nano Diamonds formed in Laser-Compressed Plastics

Thursday 23 Sep 17:00

B. Heuser[1,2], A. Schuster[2] , M.G. Stevenson[1], L. Zinta[1], Z. He[1,2], D. Ranjan[1,2], A. Ravasio[3], D. Kraus[1,2]

[2]Institut für Physik, Universität Rostock, Rostock, Germany.
[2]Institut für Strahlenphysik, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany.
[3]Laboratoire LULI, Ecole Polytechnique, Palaiseau, France.

The extreme pressure and temperature conditions found in the icy giant planets, Neptune and Uranus, can be reproduced using laser-driven shock compression. The conditions persist on nanosecond timescales and can be investigated using in situ ultra-bright and ultra-short X-ray pulses [1]. They are particularly interesting due to the failure of classical condensed matter and ideal plasma theory and the chemistry of these conditions is poorly understood [2]. The interior of these planets are mainly composed of a mixture of water, methane and ammonia [3]. When reproducing these pressure and temperature states via laser-driven shock compression of polystyrene (C8 H8)n the formation of diamond has been observed [4]. This nano diamond (ND) formation has been reported in laboratory experiments utilising laserdriven shock waves which reach pressures in the range of ∼150 GPa and ∼5000 K [5]. The formation process itself is not yet completely understood. Ongoing efforts use in situ VISAR, SOP, XRD and SAXS measurements to shed light on the underlying mechanisms and the role of different atomic mixtures, especially the influence of oxygen. It is suggested that the possible insulator-metal transition of hydrogen expected in this regime may play a key role. Since the NDs are ejected at hyper-velocities (∼10 km/s) and as part of a debris cloud, their intact recovery is a challenging task. Furthermore, the amount of diamond material is estimated to lie in the tens of microgram regime. Numerous catcher designs based on a variety of materials were tested in previous recovery experiments. Preliminary analysis showed promising structures. First insights into the temo-spatial dynamics of the ejecta cloud were obtained using ultra high speed optical imaging. Furthermore, post-analysis of captured material using spectroscopy, microscopy, diffraction and chemical methods have already provided better understanding of the challenges that still need to be overcome. Most recent data from an upcoming recovery campaign at LULI in September this year will be presented. The pressure states probed in this experiment will range up to ∼400 GPa. Its goal is the recovery from different shock-compressed plastics using the so far most promising and one completely

new catcher design. Post analysis may reveal the processes driving the diamond formation at differing H-C-O ratios. This may also provide crucial insights into the chemistry of those mixtures at planetary interior conditions.

[1] D. Kraus et al. "High-pressure chemistry of hydrocarbons relevant to planetary interiors and inertial confinement fusion". In: Physics of Plasmas 25.5 (May 2018), p. 056313.
[2] Frank Graziani et al., eds. Frontiers and Challenges in Warm Dense Matter. en. Vol. 96. Lecture Notes in Computational Science and Engineering. Cham: Springer International Publishing, 2014.
[3] Tristan Guillot. "THE INTERIORS OF GIANT PLANETS: Models and Outstanding Questions". In: Annual Review of Earth and Planetary Sciences 33.1 (2005), pp. 493–530.
[4] D. Kraus et al. "Formation of diamonds in lasercompressed hydrocarbons at planetary interior conditions". In: Nature Astronomy 1.9 (Sept. 2017), pp. 606–611.
[5] A. K. Schuster et al. "Measurement of diamond nucleation rates from hydrocarbons at conditions comparable to the interiors of icy giant planets". In: Physical Review B 101.5 (Feb. 2020), p. 054301.
email: benjamin.heuser@uni-rostock.de

Thursday
23 Sep
17:00

Diamond Formation in Laser Compressed Plastics

L.M.V. Zinta[1], M.G. Stevenson[1] , B. Heuser[1], Z. He[1], D. Ranjan[1], M. French[1], A. Bergermann[1], T.E. Cowan[2], O. Humphries[2], J. Lütgert[2], K. Voigt[2], A. Schuster[2], F. Lefevre[3], T. Vinci[3], B. Nagler[4], H.J. Lee[4], D. Khaghani[4], E. Galtier[4], E.E. McBride[4], N.J. Hartley[4], A.E. Gleason-Holbrook[4], S.H. Glenzer[4], S. Pandolfi[4], A. Descamps[4], B. Ofori-Okai[4], C. Schoenwaelder[4], G. Glenn[4], L. Fletcher[4], R. Redmer[1], A. Ravasio[3], D. Kraus[1,2]

[1]Universität Rostock, Rostock, Germany
[2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany
[3]Laboratoire LULI, Ecole Polytechnique, Palaiseau, France
[4]SLAC National Accelerator Laboratory, Menlo Park, USA Neptune and Uranus – the ice giants – are the outermost planets of our solar system. Over the last decade, the space missions CoRoT from ESA and Kepler from NASA found great variety in the possible internal structures of extrasolar planets. Ice giant planets are by far the most often discovered planets until now [1]. Models propose that the planet's mantle layer mainly consists of water, ammonia, and methane. Under the planetary interiors' pressure and temperature conditions, the constituents undergo phase transitions and even more severe chemical reactions. Therefore, it is a significant challenge to understand such mixtures' physical and chemical behavior under temperature-pressure conditions as relevant for ice giant planets like Neptune and Uranus. Demixing of hydrocarbons leads to the formation of diamonds and precipitation of the nucleates towards the planetary core [2, 3]. The remaining hydrogen becomes metallic and would contribute to currents that might explain the non-axial, non-dipolar magnetic fields [4]. Gibbs-ensemble Monte Carlo simulations have already shown demixing for helium-hydrogen mixtures under high pressure

and temperature conditions [5]. However, adopting the method to a 1:1 mixture of carbon and hydrogen did not result in a demixed system for the investigated pressures and temperatures ($\leq$60 GPa, $\leq$3000 K). Further theoretical approaches to CH-demixing need more advanced potentials or rather potentials that well depict the high-pressure interactions. In our experiment carried out at the MEC end station at the LCLS XFEL in December 2020, thin plastic samples resembling different C:H:O stoichiometries were used to study the influence of oxygen on the formation of diamond. A high-power drive laser induced a shock wave into the sample, compressing it to high pressure and temperature. Different diagnostics like X-Ray Diffraction (XRD), Small Angle X-Ray Scattering (SAXS) and velocity interferometry with a VISAR system provide insight into the dynamic evolution of the samples during compression. Approximate conditions can be estimated with hydrodynamic simulations using the equation of state (EoS) of the specific material. EoS data for several C:H:O stoichiometries have been used to estimate the P-T conditions initially. Improvements to the plastics EoS are ongoing. From the VISAR shock travel time, we found the pressures of shock compressed PLA ($C_3H_4O_2$) to be in a range of 60 - 180 GPa depending on the laser intensity. Initial analysis of the diffraction has suggested the presence of the (111) and (220) diamond reflections for low and moderate drive intensities. However, the highest drive intensity shots noticeably lacked evidence of diamond formation, likely due to increasing temperature. Ongoing work with the diffraction aims to calculate diamond crystallite sizes and nucleation rates [6].

[1] Horner, J. et al. PASP 132, 102001 (2020).
[2] Ross, M. Nature 292, 435–436 (1981).
[3] Kraus, D. et al. Phys. Plasmas 25, 056313 (2018).
[4] Redmer, R., Mattsson, T. R., Nettelmann, N. French, M., Icarus 211, 798–803 (2011).
[5] Bergermann, A., French, M., Schöttler, M Redmer, R., Phys. Rev. E 103, 013307 (1 2021)
[6] Schuster, A. K. et al. Phys. Rev. B 101, 054301 (2020).

The work was supported by the Helmholtz Association under VH-NG-1141 and ERCRA-0041. Use of the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515. The MEC instrument is supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences under Contract No. SF00515.

email: lisa.zinta@uni-rostock.de

Emission and Reflectivity of the Shock Compressed Silicon Plasma

Thursday 23 Sep 17:00

M. I. Kulish, D. N. Nikolaev, S. V. Dudin. V. B. Mintsev, I. V. Lomonosov, V. E. Fortov

Institute of Problems of Chemical Physics RAS, 142432, Chernogolovka, Russia

Direct measurements of radiation from the shock wave front provide important information about the temperature of the shock-compressed matter and, therefore, together with measurements of kinematic parameters of its propagation, determine thermodynamically complete equation of state of the matter under conditions of high dynamic pressures. Measuring the temperature of the shock wave front is possible in matters that are transparent for the range of radiation under study. To determine the temperature of a shock-compressed matter, the measurement of the emission of the shock front should be accompanied by the measurement of the shock wave reflection coefficient. In this work we measured the radiation intensity and reflectivity of the shock compressed silicon samples in the pressure range of 68-98 GPa. Reflection coefficients were measured at five wavelengths covering the range of strong absorption of radiation of silicon samples $0.74< \lambda <0.97\mu$m and at two wavelengths $\lambda = 1.3\mu$m and $\lambda = 1.5\mu$m, in the range where absorption is small for the characteristic thicknesses of samples $d \sim 1$mm. We measured the radiation intensity of silicon samples in two wide spectral ranges $\Delta\lambda_1 = (0.32 \pm 1.06)\mu$m and $\Delta\lambda_2 = (1.1 \pm 1.7)\mu$m in which the first range of silicon absorbs radiation at a thickness d, while the second range of silicon sample is transparent. It was found that the reflection coefficient from the shockwave front R$\sim$0.1 and the brightness temperature of the shock front T=1250 K. The analysis of measurement results and comparison of obtained values of brightness temperatures of the radiation front with calculations according to the equations of state allows us to conclude that the radiation of the shockcompressed silicon is screened by the absorbing layer propagated before shock front.

Local field correction to ionization potential depression of ions in warm/hot dense matter

Thursday 23 Sep 17:00

Xiaolei Zan[1], Chengliang Lin[2], Yong Hou[1] and Jianmin Yuan[1,2]

[1]Department of Physics, College of Liberal Arts and Sciences, National University of Defense Technology, Changsha, Hunan 410073, Peoples Republic of China

[2]Graduate School of China Academy of Engineering Physics, Beijing 100193, Peoples Republic of China

An analytical self-consistent approach was recently established to predict the ionization potential depression (IPD) in multi-component dense plasmas, which is achieved by considering the self-energy of ions and electrons within the quantum statistical theory [1,2]. In order to explicitly account for the exchange-correlation effect of electrons, we incorporate the effective static approximation of local field correction (LFC) [3] within our IPD framework through the connection of dynamical structure factor. The effective static approximation poses an accurate description for the

asymptotic large wave number behavior with the recently developed machine learning representation of static LFC induced from the path-integral Monte Carlo data [4]. Our calculation shows that the introduction of static LFC through dynamical structure factor brings a non-trivial influence on IPD at warm/hot dense matter conditions. The correlation effect within static LFC could provide up to 20% correction to free-electron contribution of IPD in the strong coupling and degeneracy regime. Furthermore, a new screening factor is obtained from the density distribution of free electrons calculated within the average-atom model [5], with which warm dense Fe plasmas and Mg plasma were studied in detail. Full version of IPD calculations on Fe plasmas were performed at a wide range of density-temperature conditions, and excellent agreements are obtained with the commonly employed SP or EK model at their corresponding validly regime. Additionally, our IPD calculation matches perfectly with the experiment result [6] performed on Mg plasma at $n_e = 3.0 \times 10^{23}\text{cm}^{-3}$ and $T = 75$ eV.

[1] C. Lin, G. Röpke, W. D. Kraeft, and H. Reinholz. Ionization-potential depression and dynamical structure factor in dense plasmas. Phys. Rev. E 96, 013202 (2017).
[2] C. Lin. Quantum statistical approach for ionization potential depression in multicomponent dense plasmas. Phys. Plasmas 26, 122707 (2019).
[3] T. Dornheim, A. Cangi, K. Ramakrishna, M. Bohme, S. Tanaka, and J. Vorberger. Effective static approximation: A fast and reliable tool for warm-dense matter theory. Phys. Rev. Lett. 125, 235001 (2020).
[4] T. Dornheim, J. Vorberger, S. Groth, N. Hoffmann, Z. A. Moldabekov, and M. Bonitz. The static local field correction of the warm dense electron gas: An ab initio path integral monte carlo study and machine learning representation. J. Chem. Phys. 151, 194104 (2019).
[5] Y. Hou, R. Bredow, J. Yuan, and R. Redmer. Average-atom model combined with the hypernetted chain approximation applied to warm dense matter. Phys. Rev. E 91, 033114 (2015).
[6] Q. Y. van den Berg, E. V. Fernandez-Tello, T. Burian, J. Chalupsky, H. K. Chung, O. Ciricosta, G. L. Dakovski, V. Hajkova, P. Hollebon, L. Juha, J. Krzywinski, R. W. Lee, M. P. Minitti, T. R. Preston, A. G. de la Varga, V. Vozda, U. Zastrau, J. S. Wark, P. Velarde, and S. M. Vinko. Clocking femtosecond collisional dynamics via resonant x-ray spectroscopy. Phys. Rev. Lett. 120, 055002 (2018).
EMAIL: jmyuan@nudt.edu.cn

Criteria for locating the melting and crystallization points of 2D strongly coupled Coulomb systems

Thursday
23 Sep
17:00

Ye. K. Aldakul

Institute of Applied Sciences and IT, 40-48 Shashkin Str., 050038 Almaty, Kazakhstan

In order to locate the melting points of 2D crystal structures one usually computes an orientational order parameter (OOP). For a triangular lattice the OOP is defined as follows [1]

$$\Psi_j = \frac{1}{N_j} \sum_{k}^{N_j} \exp(6i\theta_{jk}) \tag{1}$$

where N_j is the number of the nearest neighbor particles, i is the imaginary unit, and θ_{jk} is the angle between the x-axis and a bond connecting particles j and k. A universal criteria for locating the melting point of 2D systems is to look for the value of the overall OOP, $\Psi_0 = |\langle\Psi_j\rangle|$ The melting of the system occurs when $\Psi_0 \sim 0.45$ [2]. However, in our MD simulations of 2D electric dipoles we found that this melting criteria fails to locate the crystallization point, the value of Ψ_0 stayed well below the 0.45 value even when the system had crystallized [3]. The reason for the low values of Ψ_0 was due to the presence of domains with different orientations of Ψ_j, which cancel each-other in averaging process. Therefore, to locate the crystallization point we computed the local OOP, $\Psi_l = \langle|\Psi_j|\rangle$, and found that the crystallization as well as melting of the system occurs when $\Psi_l \sim 0.67$. In addition, we implemented the polygon construction method [4] and located the same phase transition points by looking for the value of 0.165 of a polygon disorder parameter. Also, we found that these values of Ψ_l and the polygon disorder parameter are independent of the screening in the potential, and we expect that the obtained values are universal for other 2D systems with a repulsive pair potential. Thus, $\Psi_l \sim 0.67$ and the value of 0.165 of a polygon disorder parameter can serve as two additional criteria to investigate the melting and crystallization of 2D systems with repulsive interaction potentials.

[1] B. I. Halperin and D. R. Nelson, Phys. Rev. Lett. 41, 121 (1978).
[2] I. V. Schweigert, V. A. Schweigert, and F. M. Peeters, Phys. Rev. Lett. 82, 5293 (1999).
[3] Ye. K. Aldakul, Zh. A. Moldabekov and T. S. Ramazanov, Phys. Rev. E 102, 033205 (2020)
[4] M. A. Glaser and N. A. Clark, Adv. Chem. Phys. 83, 543 (1993).

Thursday
23 Sep
17:00

Electronic stopping in warm dense matter using Ehrenfest dynamics and time-dependent density functional theory

Andrew D. Baczewski, Alina Kononov, Thomas Hentschel, Stephanie Hansen
Sandia National Laboratories

Ehrenfest dynamics with time-dependent density functional theory (TDDFT) provides a framework for first principles calculations of electronic stopping power that has been successfully applied in the solid state in numerous contexts. Its use in the warm dense regime has not been as widely studied, in part thanks to the computational expense of treating a large number of thermally occupied orbitals. In this contribution we will examine some of the challenges associated with scaling Ehrenfest+TDDFT into the warm dense regime. We first consider isochorically heated aluminum, which allows us to study the impact of the pseudization of the L-shell under conditions in which it is increasingly thermally depleted. We then consider all-electron calculations of liquid-like deuterium and carbon to study the impact of finite-size effects and configurational averaging as a function of projectile energy. We conclude by taking the lessons we have learned to the analysis of electronic stopping in deuterium/beryllium mixtures relevant to fusion experiments. Throughout, we

work within the context of validating average-atom models for the elemental systems and providing benchmark data for mixtures. We also report on some of the computational aspects of these calculations, which are among the largest of their kind.
SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

Stopping in dense quantum plasmas using a new Greens Functions approach

Thursday
23 Sep
17:00

Christopher Makait, Francisco Borges Fajardo, Niclas Schlünzen, Jan-Philip Joost, Michael Bonitz

Christian-Albrechts Universität Kiel, Germany

Quantum kinetic approaches [1] have proven successful in describing the dynamics of the uniform electron gas (UEG) and quantum plasmas. The Nonequilibrium Green Functions (NEGF) method is a powerful tool to compute time-dependent expectation values of single-particle observables in correlated quantum many-body systems, however, it his hampered by an unfavorable N_t^3-scaling with propagation time N_t. This scaling can be reduced to N_t^2 by introduction of the Generalized Kadanoff-Baym Ansatz (GKBA) for simple second order Born selfenergies [2]. Recently, an exact time-local (N_t^1) reformulation of the GKBA, the G1–G2 scheme [3,4], has been found for various self energies, which makes this method viable for long time simulations.

In standard NEGF simulations of homogeneous quantum plasmas the inclusion of exchange diagrams is significantly more involved than direct diagrams that can be treated by fast Fourier transform methods. In the G1–G2 scheme they are equally expensive to compute, making this method especially efficient when considering exchange diagrams and advanced selfenergies such as the dynamically screened ladder approximation.

In this poster we present the first time-resolved results for ion and electron stopping in two-component quantum plasmas extending earlier Lenard-Balescu simulations [5]. First, we test the G1–G2 scheme for the model of a 1D plasma. Second, we apply the standard GKBA to the stopping in 3D plasmas.

[1] M. Bonitz, *Quantum Kinetic Theory* (Springer, 2016)
[2] P. Lipavský, V. Špička, and Velický, B, Generalized Kadanoff-Baym ansatz for deriving quantum transport equations, *Phys. Rev. B* **34**, 6933 (1986)
[3] N. Schlünzen, J.-P. Joost, M. Bonitz, Achieving the Scaling Limit for Nonequilibrium Green Functions Simulations, *Phys. Rev. Lett.* **124**, 076601 (2020)
[4] J.-P. Joost, N. Schlünzen, M. Bonitz, The G1–G2 Scheme: Dramatic Acceleration of Nonequilibrium Green Functions Simulations Within the Hartree–Fock-GKBA, *Phys. Rev. B* **101**, 245101 (2020)
[5] M. Bonitz, D. Kremp, S. Kosse, D. C. Scott, W. D. Kraeft, *Influence of many-particle effects on stopping power.* In: Proceedings of the International Conference on the Physics of Strongly Coupled Plasmas, Sept. 11-15 1995, Binz, Eds. W. D. Kraeft, M. Schlanges, World Scientific 1996

Ion impact on strongly correlated 2D materials — stopping power and induced collective electronic dynamics

Thursday 23 Sep 17:00

Franziska Reiser, Lotte Borkowski, Jan-Philip Joost, Niclas Schlünzen, Michael Bonitz

Kiel University

The energy loss of charged projectiles in correlated materials is of prime relevance for plasma-surface interaction for which we have developed a nonequilibrium Green functions (NEGF) approach. Some particularly interesting effects that occur when a charged plasma particle hits a strongly correlated solid are the correlation induced increase of stopping power at low velocities [1] as well as the creation of doublons (bound correlated pairs of electrons with opposite spins). However, NEGF simulations are possible only for short time durations, due to the unfavorable N_t^3 scaling with the number of discretization time steps. This situation has changed radically with the recently developed G1-G2 scheme [2], which is based on the generalized Kadanoff-Baym ansatz in combination with Hartree-Fock propagators, and allows us to achieve linear scaling with N_t . This enables us to study larger finite systems of varying geometry and to significantly extend the simulation duration which gives access, in particular, to slower projectiles. Furthermore, it enables us to improve the accuracy by using better self-energies that include dynamical screening and strong coupling effects simultaneously [3]. In addition, the systematic increase of the doublon number through multiple projectile impacts [4] is investigated for more realistic setups (e.g. larger systems and random projectile impact points).

[1] Balzer et al., Phys. Rev. B 94, 245118 (2016)
[2] Schlünzen et al., Phys. Rev. Lett. 124, 076601 (2020)
[3] Joost et al., Phys. Rev. B 101, 245101 (2020)
[4] Balzer et al., Phys. Rev. Lett. 121, 267602 (2018)

Electron mean free path and the Dreicer field in dense semiclassical plasma

Thursday 23 Sep 17:00

M.M. Seisembayeva[1], E.O. Shalenov[1,2] and K.N. Dzhumagulova[1,2]

[1]Institute of Experimental and Theoretical Physics, al-Farabi Kazakh National University, Almaty, 050040, Kazakhstan

[2]Department of Physics, Nazarbayev University, Nur-Sultan, 010000, Kazakhstan

High-energy electrons appear in plasma, for example, in thermonuclear devices, solar flares, laser plasma, energy discharges associated with thunderstorms. One of the important mechanisms for the appearance of such suprathermal electrons is the electron runaway phenomenon in an external electric field. Runaway electrons play a positive role in the case of wake acceleration, inertial confinement fusion (ICF) fast ignition, etc., however, can be a big problem, namely, by its uncontrollability, which leads, for example, to a damage of the walls in the thermonuclear installations. Therefore, an understanding of the runaway mechanism and knowledge of the dynamics of runaway electrons are crucial in order to control this phenomenon. In

this work, the phenomenon of electron runaway in dense semiclassical plasma was investigated on the basis of the effective interaction potential, which takes into account the effects of dynamic screening and diffraction [1–2]. Plasma was considered to be fully ionized, i.e. the electron-electron and electron-ion interactions are only taken into account. The calculations were carried out using the method of phase functions. The electron transport cross sections were calculated, and on their basis the mean free path of electrons was determined for various values of the density and coupling parameters. Critical external electric field (the Dreiser field) which is one of the important characteristic of the runaway phenomenon was also investigated.

[1] Dzhumagulova K.N. etc. al. Phys. Plasmas. – 2013. – Vol. 20. – p. 042702.
[2] Shalenov E.O. etc. al. Phys. Plasmas. – 2018. Vol. 25. – p. 082706.

The authors acknowledge support from the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan under Grant number AP08855972.

e-mail: Shalenov.erik@mail.ru

Strongly increasing electron-impact-ionization cross section in hot dense plasma by the ion correlation effect and continuous electron decoherence

Thursday
23 Sep
17:00

Ping Zhang[1], Yang Jin[1], Xiaolei Zan[1], Yong Hou[1], and Jianmin Yuan[1,2]

[1] Department of Physics, College of Liberal Arts and Sciences, National University of Defense Technology, Changsha Hunan 410073, People's Republic of China;
[2]Graduate School, China Academy of Engineering Physics, Beijing 100193, People's Republic of China

There are significant discrepancies between the recent experiment (Berg et al, Phys. Rev. Lett. 120, 055002) and current theoretical calculations on the electronimpact ionization in hot dense plasmas. For the theoretical results are based on structures of the isolated atoms of ions, without considering the influence of hot dense plasmas, we present a model to consider the effects of the ion and free electrons in the self-consistently calculations of ionic structures, and free electrons decoherence in the electron-impact ionization. The correlation effects due to the interactions between ions and surrounding free electrons, are included by the correlation functions, which are calculated by hyper-netted chain (HNC) approximation. And the effect yields an additional Hermitian potential to the atomic central potential, and will significantly change the atomic structure compared with that of the isolated ion. Due to the partial decoherence caused by random collision with free electrons and ions, we use damped plane waves of the scattered electrons instead of plane waves, which considers the influence of hot dense plasma on the electron collision process. Finally, we study the electron-impact ionization process of Mg7+ in solid-density plasma using the theoretical model, which result in the increase of the ionization cross section by one order of magnitude compared with that of the isolated ion, And the result is an excellent agreement with the experimental result of Berg et al. The model shed some new insights on collisional ionization process, and would be used to study the radiation opacity and the nonequilibrium properties of hot dense plasma.

email: yonghou@nudt.edu.cn

Thursday
23 Sep
17:00

Transport properties of inertial confinement fusion dense plasmas

Kodanova S.K., Ramazanov T.S., Issanova M.K.

IETP, Al-Farabi Kazakh National University, Almaty, Kazakhstan, Al-Farabi av., 71

Studying of transport properties of the dense plasma is a great importance for plasma physics, as well as for the problems of inertial confinement fusion (ICF), warm dense matter driven by heavy ion beams [1]. Calculation of parameters of inertial fusion drivers $n_e = 10^{22}\text{cm}^{-3}$ heavy ion beams requires adequate quantitative description of the interaction of heavy ion beams with dense plasma in a wide range of parameters. Consequently, knowledge of transport properties in the plasma will enable us to calculate the design of thermonuclear target more accurately. These properties of plasma can be calculated accurately taking into account both quantum and collective effects in plasmas. One of the important values describing the transport coefficients of deuterium-tritium plasma is the Coulomb logarithm [2]. The Coulomb logarithm is obtained on the basis of effective potentials. These interaction potentials take into consideration long-range many particle screening effects as well as short-range quantum-mechanical effects [3]. For inertial confinement fusion applications, we have calculated deuterium thermal conductivity and electrical conductivity in a wide range of densities and temperatures. The results obtained for thermal conductivity and electrical conductivity are compared with the available experimental data [4] and the results of quantum molecular-dynamics simulation [5].

[1] V.E. Fortov. Extreme states of matter on Earth and in the Cosmos. – Springer, 2009

[2] T.S. Ramazanov, S.K. Kodanova, Zh.A. Moldabekov, M.K.Issanova. Phys. Plasmas, 2013, 20, P. 112702.

[3] S.K. Kodanova, T.S. Ramazanov, M.K. Issanova, Zh.A. Moldabekov, G. Nigmetova. Contrib. Plasma Phys., 2015, 55 (2-3), pp 271 – 276.

[4] J.R. Adams, N.S. Shilkin, V.E. Fortov, V.K. Gryaznov, V.B. Mintsev, R. Redmer, H. Reinholz, and G. Röpke. Phys. Plasmas, 2007, 14, P. 062303.

[5] S.X. Hu, L.A. Collins, T.R. Boehly, J.D. Kress, V.N. Goncharov and S. Skupsky. Phys. Rev., 2014, E 89, P. 043105.

email: isanova_moldir@mail.ru

Dissociation of quarkonium in collisional quark-gluon plasma

Thursday 23 Sep 17:00

Y. Kuanyshbaiuly[1,2], K.M. Baiseitov[1,2], T.S. Ramazanov[1]

[1]Institute for Experimental and Theoretical Physics, Al-Farabi Kazakh National University str., 050040 Almaty, Kazakhstan

[2]Institute of Applied Science and IT, 40-48 Shashkin Str., 050038 Almaty, Kazakhstan

Quark-gluon plasma (QGP) is state of highly dense matter at extreme temperature, which consists of stronginteracting quarks and gluons governed by quantum chromodynamics (QCD). Production of QGP can be achieved in relativistic heavy ions collision experiments such as CERN SPS and BNL RHIC. One of the main signals of quark-gluon plasma formation in heavy ion collisions is suppression of quarkonium [1]. Quarkonium is meson composed of heavy quark-antiquark pair of same flavour, namely charm and bottom quark. They usually referred to as J/Ψ and Υ mesons. Heavy quark systems are of particular interest, because they form very compact bound states comparing to ordinary matter baryons and mesons, so that they survive QGP phase transition, where the latter ones undergo deconfinement due to Debye screening length. As temperature and density of matter increase the J/Ψ and Υ mesons also dissociate. Bound states can be studied using effective confined potential in framework of non-relativistic model [2]. The ground state energies and radii for charmonium and bottomonium were calculated using numerical method for solving Schrodinger equation with potential modified for dynamical screening case [3]. Potential is described by dielectric function for QGP [4], which takes into account pair interaction by Bhatnagar-Gross-Krook collision operator. The production of quarkonia suppresses at the specific values of screening radius, which is calculated in this work.

[1] T. Matsui, H. Satz, Phys. Lett. B 178, 416 (1986).

[2] F. Karsch, M. T. Mehr, H. Satz, and Z. Phys. C37(4), 617-622(1988).

[3] Zh. A. Moldabekov, P. Ludwig, J.-P. Joost, M. Bonitz, and T. S. Ramazanov, Contrib. Plasma Physics 55, 186-191 (2015).

[4] P. Chakraborty, M. G. Mustafa, R. Ray, and M. H. Thoma, J. Phys. G: Nucl. Part. Phys. 34, 2141(2007).

Scaling EUV and X-ray Thomson Scattering Sources to Optical Free-Electron Laser Operation using Traveling-Wave Thomson-Scattering

Thursday 23 Sep 17:00

Alexander Debus[1], Klaus Steiniger[1], Daniel Albach[1], Michael Bussmann[1,3], Markus Löser[1], Richard Pausch[1], Fabian Röser[1], Mathias Siebold[1], Ulrich Schramm[1,2]

[1]Helmholtz-Zentrum Dresden Rossendorf (HZDR), Dresden, Germany

[2]Technische Universität Dresden, Dresden, Germany

[3]Center for Advanced Systems Understanding (CASUS), Görlitz, Germany

Traveling-Wave Thomson-Scattering (TWTS) is a novel Thomson scattering geometry which allows for orders of magnitude higher photon yields than classic head-on Thomson sources. TWTS thereby remains compact and provides narrowband and

ultra-short ultraviolet to γ-ray radiation pulses just as classic Thomson sources. Even the realization of optical free-electron lasers (OFELs) is possible with the TWTS geometry since it provides both optical undulators with thousands of periods needed to microbunch the electron beam and a reduction of electron beam quality requirements compared to classic Thomson scattering to a level technically feasible today. TWTS employs a side-scattering geometry in which laser and electron propagation direction of motion enclose the interaction angle ϕ. Tilting the laser pulse front with respect to the wave front by half the interaction angle ensures continuous overlap of electrons and laser pulse over the whole laser pulse width while the laser pulse crosses the electron beam trajectory. In this way the interaction length becomes controllable by the laser pulse width and independent of the laser pulse duration. Utilizing wide, petawatt class laser pulses for TWTS allows to realize thousands of optical undulator periods. The variability of TWTS with respect to the interaction angle can be used to control the radiation wavelength even for electron sources with fixed energy. For a fixed target wavelength on the other hand, the free choice of interaction angle enables control over electron beam quality requirements. Small interaction angle scenarios ($\phi \sim 10^\circ$) typically yield the best trade-off between requirements on electron beam quality, laser power and laser intensity stability. We will show that TWTS OFELs emitting extreme ultraviolet radiation are realizable today with existing technology for electron accelerators and laser systems. We detail an experimental setup to generate the tilted TWTS laser pulses which aims at compactness and provides focusing of these highpower pulses and compensation of dispersion accompanying pulse-front tilts. The method presented for dispersion compensation is especially relevant when building high yield X- and γ-ray sources in large interaction angle setups of TWTS.

Surrogate Modelling of Ion Acceleration and Overdense Laser-Plasma Interactions

Thursday
23 Sep
17:00

Thomas Miethlinger
HZDR

The interaction of overdense plasma with ultra-intense laser pulses presents a promising approach to enable the development of very compact ion sources. Prospective applications of high-energetic protons and ions include, but are not limited to, medical applications (in particular ion beam radiotherapy), laboratory astrophysics and nuclear fusion. However, current records for maximum proton energies (94 MeV, 2018) are still below the required values for the aforementioned applications (typically in the range of 150-250 MeV), and especially challenges such as stability and spectral control remain unsolved to this day. In particular, significant effort per experiment and a high-dimensional design space renders naive sampling approaches ineffective. Furthermore, due to the strong nonlinearities of the underlying laser-plasma physics, synthetic observations by means of particle-in-cell (PIC) simulations are computationally very costly, and the maximum distance between two sampling points is strongly limited as well. Consequently, in order to build useful surrogate models for future data generation and experimental understanding and control, a

combination of highly optimized simulation codes (where we employ PIConGPU), powerful data-based methods, such as artificial neural networks (ANNs), and modern sampling approaches are essential. Specifically, we employ invertible neural networks for bidirectional learning of input (parameter) and output (observables) and convolutional autoencoder to reduce intermediate field data to a lower-dimensional latent representation.

The effect of nanoparticles to plasma emission intensity of the RF discharge

Thursday
23 Sep
17:00

Orazbayev S.A.[1], Zhumadilov R.E.[1], Utegenov A.U.[1], Gabdullin M.T.[2], Ramazanov T.S.[1]

[1]Al-Farabi Kazakh National University, Almaty, Kazakhstan
[1]Kazakh-British Technical University, Almaty, Kazakhstan

Gas discharge lighting devices are considered a simple device in everyday life. The growing value of energy and maintenance, the need for environmentally friendly systems, the need to reduce energy consumption and, consequently, greenhouse gas emissions, make the continuous development of existing and future light sources necessary. In many cases, the used lighting technologies based on materials such as gotters, working amalgams and starting amalgams, which improve the performance of gas-discharge light sources and allow the production of light sources with superior performance and greater efficiency [1]. This paper is devoted to experimental investigations of the carbon nanoparticles growth process in RF discharge of argon-methane gas mixture. In particular, the dependence of nanoparticle nucleation time on gas discharge parameters was investigated by observing the self-bias voltage [2]. Furthermore, a detailed analysis of the synthesized nanoparticles was carried out to determine the size by SEM for each time point from 0 to 35 seconds at different discharge parameters such as power and pressure. More importantly, the discharge was found to change the emission property depending on the size of the nanoparticles at certain parameters of the plasma with nanoparticles. In order to understand this phenomenon in more detail, experiments were carried out to study the dependence of plasma volume glow intensity on various gas discharge parameters (percentage of plasma-forming gas mixture, pressure in the working volume and discharge power). Eventually, the optimum nanoparticle sizes and discharge conditions at which maximum plasma glow can be achieved were determined.

[1] Alessio Corazza, Stefano Giorgi, and Vincenzo Massaro “Materials to Improve Performance of Discharge Lamps” // IEEE TRANSACTIONS ON INDUSTRY APPLICATIONS, VOL. 48, NO. 5, 2012, P. 1668-1672.

[2] Influence of Gas Temperature on Nucleation and Growth of Dust Nanoparticles in RF Plasma// IEEE Transactions On Plasma Science. 2019. – Vol. 47(7). - P. 3069.

Thursday
23 Sep
17:00

Charging of Dust Particles in Space Plasma in the Presence of Suprathermal Electrons

M. Myrzaly, R. U. Masheyeva, K. N. Dzhumagulova

IETP, Al-Farabi Kazakh National University, 71 Al-Farabi av., Almaty 050040, Kazakhstan

It has now been stated that most of the space plasma is the so-called plasma with a condensed dispersed phase, or dusty plasma [1]. Dusty plasma is present in planetary rings, comet tails, interplanetary space and interstellar clouds. The sizes of dust particles range from a fraction to several micrometers. Due to these sizes, such particles can acquire very large static electric charges due to the flow of ions and electrons onto their surface. To describe the process of charging dust grains, the so-called method of the orbit motion limited (OML) approximation, is widely used. In the well-known equations obtained on the basis of this method, the equilibrium Maxwell distribution was initially used. Meanwhile, spacecraft measurements have shown that deviations from the equilibrium distribution of plasma particles are often found in the solar wind, in the plasma of planetary magnetospheres and some other astrophysical objects due to the presence of high-energy particles [2]. In most cases, the distribution has a power-law tail at high energies. As has been shown, the best fit to the available empirical data is the so-called family of κ (kappa) distributions. At present, it has already found the interesting applications in dusty plasma physics. For example, in Ref.[3], dust-acoustic solitons in dusty plasma with k-distributed ions were investigated. In the presented work, we obtained expressions for the fluxes of plasma particles onto the surface of dust particles based on the kappa - distribution of background plasma particles and solved the equations describing the charging of dust grains in nonequilibrium space plasma. A detailed analysis of the results obtained in a wide range of changes in the parameters of the system and the kappa distribution is made.

[1] Goertz C.K. Dusty plasmas in the solar system // Rev. Geophys, 27, 271–292 (1989).

[2] Livadiotis, G. Introduction to special section on origins and properties of kappa distributions: statistical background and properties of kappa distributions in space plasmas // J. Geophys. Res. Space Physics, 120, 10.1002/2014JA020825 (2015).

[3] T. K. Baluku and M. A. Hellberg. Ion acoustic solitons in a plasma with twotemperature kappa-distributed electrons // Phys. Plasmas 19, 012106 (2012).

The authors acknowledge support from the Science Committee of the Ministry of Education and Science of the Republic of Kazakhstan under Grant number AP09058005.

e-mail: dzhumagulova.karlygash@gmail.com

Dusty plasma in a strong and sharply inhomogeneous magnetic field

Thursday
23 Sep
17:00

Karasev V.Yu., Dzlieva E.S., Pavlov S.I., Novikov L.A., Tarasov S.A, Gasilov M.A.
Saint Petersburg State University, 199034, Universitetskaya nab., 7/9, St. Petersburg, Russia

In studying of dusty plasma under the influence of a magnetic field to simplify the physical problem a homogeneous magnetic field with a degree of inhomogeneity of up to 0.01exception is work [1], but for monolayer dusty structures created under the conditions of an HF discharge, the longitudinal inhomogeneity does not have a noticeable effect. Today, experimental studies are carried out in a strong magnetic field with an induction of up to 6 T, which affects the discharge even in a uniform field [2-5]. In [6-8], bulk dusty structures were created in a strong magnetic field in a glow discharge. The use of bulk dusty structures makes it possible to place dusty plasma in a strongly inhomogeneous longitudinal magnetic field [9]. In this work, a dust structure is created in a sharply inhomogeneous magnetic field with a longitudinal gradient of 0.2 T / cm. To create a dusty structure, a glow discharge in neon at a pressure of less than 1 Torr was used and polydisperse quartz particles were used. The inhomogeneity of the magnetic field is created near the end of the superconducting solenoid, which creates a magnetic field in its center of 2 T. A significant effect of an inhomogeneous magnetic field on both the discharge and the dust trap was found. The radial and longitudinal dimensions of the dusty plasma are determined. In the longitudinal direction, dusty plasma can form dust chains up to 8 cm long. The diameter of the dusty structure has been measured for various inhomogeneities of the magnetic field. The angular velocity of rotation was recorded as a function of the magnetic field and the longitudinal coordinate. The direction of rotation is opposite to the direction of rotation of the dusty plasma in the stratum in the case of a uniform magnetic field.

[1] Konopka U., Samsonov D., Ivlev A. V., Goree J., Steinberg V., Morfill G. E. Phys. Rev. E. 61 (2000.) 1890
[2] Melzer A., Kruger H., Schutt S. and Mulsow M. Phys. Plasmas 2019. V. 26. P. 093702.
[3] Thomas E Jr, Lynch B, Konopka U, Merlino R and Rosenberg M Phys. Plasmas. 22 030701.1-4 (2015)
[4] M. Choudhary, R. Bergert, S. Mitic, M. H. Thoma, Phys. Plasmas 2020, 27, 063701
[5] Schwabe M., Konopka U., Bandyopadhyay P., and Morfill G. E. Phys. Rev. Lett. 2011. Vol. 106. P. 215004.
[6] Dzlieva E.S., Dyachkov L.G., Novikov L.A., Pavlov S.I. and Karasev V.Yu., EPL, 2018, 123, 15001.
[7] Dzlieva E.S., Dyachkov L.G., Novikov L.A., Pavlov S.I. and Karasev V. Yu., Plasma Sources Science and Technology, 2019, 28, 085020.
[8] Dzlieva E.S., Dyachkov L.G., Novikov L.A., Pavlov S.I. and Karasev V. Yu., Plasma Sources Science and Technology. 2020. 29. 085020.
[9] Dzlieva E.S., Novikov L.A., Pavlov S.I. and Karasev V. Yu., Technical Physics Letters., 46(2020)371

The work was supported RSF grant 18-72-10019
e-mail: s.i.pavlov@spbu.ru

Thursday
23 Sep
17:00

X-ray Thomson scattering spectra from DFT-MD simulations based on a modified Chihara formula

M. Schörner[1], P. Sperling[1,2], R. Redmer[1]

[1]Institut für Physik, Universität Rostock, 18051 Rostock, Germany
[2]Aible GmbH, Am Vögenteich 24, 18055 Rostock, Germany

We demonstrate a state-of-the-art approach for calculating x-ray Thomson scattering (XRTS) spectra from DFT-MD simulations based on a modified Chihara formula [1]. We compute the ionic contribution from the ion-ion structure factor [2] and the total form factor of the electrons, while utilizing the fluctuation-dissipation theorem to predict the inelastic response of the electron system including free-free, bound-free, and bound-bound transitions. As the inelastic contribution is only directly accessible in the long wavelength limit, we extend it to finite wave vectors by using the Mermin formalism with dynamic collision frequencies determined with DFTMD. We compare the collision frequencies predicted by DFT to known analytical approaches such as the Born collision frequency and the Gould-DeWitt scheme [3] and evaluate the impact their differences have on the resulting XRTS spectra for Hydrogen at various temperatures and densities in the warm dense matter regime. We also examine the applicability of this method to Aluminum and Beryllium at a few conditions in this regime. At high densities and small scattering angles, we observe significant deviations between the DFT spectra and the Born-Mermin approach which is employed by most codes that analyze x-ray Thomson scattering experiments.

[1] B.B.L. Witte et al., Phys. Rev. Lett. 118, 225001 (2017)
[2] H.R. Rüter and R. Redmer, Phys. Rev. Lett. 112, 145007 (2014)
[3] H. Reinholz et al., Phys. Rev. E 62, 5648 (2000)

The DFT-MD simulations were performed at the North-German Supercomputing Alliance (HLRN) and at the IT and Media Center of the University of Rostock.

Author Index