

Curriculum Vitae

Personal Information

Name: Attila Cangi, Ph.D.
Birth Place and Date: Rotthalmünster, Germany, 29.10.1982
Nationality: German
Languages: German (native), English (full professional proficiency)
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Current Position

Head of Department, Machine Learning for Materials Design, Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Germany (since 2024)

Academic Career

2022–2024	Helmholtz-Zentrum Dresden-Rossendorf, Germany	Head of Department (acting), Staff Scientist (permanent)
2020–2022	Helmholtz-Zentrum Dresden-Rossendorf, Germany	Staff Scientist
2019–2020	Sandia National Laboratories, Albuquerque, United States	Staff Scientist (permanent)
2017–2019	Sandia National Laboratories, Albuquerque, United States	Staff Scientist (LTE)
2011–2016	Max Planck Institute of Microstructure Physics, Halle (Saale), Germany	Postdoctoral Researcher (with E.K.U. Gross)

Education

2011	University of California, Irvine, United States	PhD in Chemistry (with K. Burke)
2006	Rutgers, The State University of New Jersey, United States	MSc in Physics
2005	University of Würzburg, Germany	<i>Vordiplom</i> in Physics

Shortlistings for Professorships

2025	Invited to professorial appointment lecture (<i>Berufungsvortrag</i>) for Full Professorship (W3) in Scientific Machine Learning	Paderborn University and Heinz Nixdorf Institute
2024	Shortlisted candidate (<i>Berufungsliste</i>) for Full Professorship (W3) in Data Driven Simulation and Analysis in Material Science (Ranked 2nd)	Saarland University and German Research Center for Artificial Intelligence
2024	Shortlisted candidate (<i>Berufungsliste</i>) for Full Professorship (W3) in Theoretical Physics (Ranked 4th)	University of Rostock

Invited Talks (*selected*)

2026	Advances in PES Exploration for Complex Materials, CECAM Workshop, Berlin, Germany
2026	APS Global Physics Summit, Symposium on Data Science, Denver, United States (declined)
2025	Theoretical Chemistry Colloquium, University of Marburg, Germany
2024	Department Seminar, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany
2024	Progress in Ensemble Density Functional Theory: Opportunities and Challenges, Durham University, Durham, United Kingdom
2024	Machine Learning in Electronic-Structure Theory, Institute for Mathematical and Statistical Innovation (IMSI), University of Chicago, United States
2024	APS March Meeting, Focus Session: Big Datasets and Big Data in Physics, Minneapolis, United States
2023	Accelerating Improvements in Density Functional Theory, CECAM Workshop, Lausanne, Switzerland
2023	TDDFT School & Workshop: Excited states and dynamics, Rutgers University, Newark, United States
2023	High Energy Density Science Seminar Series, Lawrence Livermore National Laboratory, Livermore, United States
2023	Theoretical Chemistry Seminar, Dresden University of Technology, Germany
2023	Joint Theory Seminar of European XFEL, CFEL, and the University of Hamburg, Germany
2023	Research Seminar Many-Body Theory, Kiel University, Germany
2023	Institute Seminar, Institute of Theoretical Physics, University of Wroclaw, Poland
2022	NHR-Atomistic Simulation Symposium 2022, online, Germany
2022	Research Seminar Many-Body Theory, Kiel University, Germany
2022	Big Data Analytical Methods for Complex Systems, University of Wroclaw, Wroclaw, Poland
2022	Helmholtz AI Conference 2022, Dresden, Germany
2021	CFEL-DESY Theory Seminar, Hamburg, Germany

2021	8th International Symposium on Optics & its Applications, Rostock, Germany
2021	17th Conference on the Physics of Non-Ideal Plasmas, Dresden, Germany
2021	Supercomputing Frontiers Europe 2021, online
2019	Workshop on the Future of Uncertainty Quantification and Multiscale Modeling Across the Department of Energy, Sandia National Laboratories, Albuquerque, United States
2019	Machine Learning R&D Workshop Sandia National Laboratories, Albuquerque, United States
2019	Z Fundamental Science Workshop, Sandia National Laboratories, Albuquerque, United States
2019	10th International Workshop on Warm Dense Matter, Travemünde, Germany
2019	Computational Modeling for High Energy Density Science and Complex Systems, City University of New York, Department of Physics, New York, United States
2019	Improving the Theory in Density Functional Theory, CECAM Workshop, EPFL Lausanne, Switzerland
2018	Electronic Structure at the Cutting Edge with ELK, MPI of Microstructure Physics, Halle, Germany
2017	Teaching the Theory in Density Functional Theory, CECAM School, EPFL Lausanne, Switzerland
2015	Theoretical Physics Seminar, University of Rostock, Germany

Third-Party Funded Projects

2026–2029	Helmholtz AI, Helmholtz Association, Germany	Machine Learning Green Functions for Magnetic Materials and Spintronics
2026–2029	Federal Ministry for the Environment, Climate Action, Nature Conservation and Nuclear Safety (BMUKN), Germany	Machine Learning for Complex Hydrological–Geochemical Processes in Crystalline Rock Disposal
2021–2024	Helmholtz AI, Helmholtz Association, Germany	Machine-Learning Based Synthetic Data Generation For Rapid Physics Modeling
2019–2022	Department of Energy, LDRD (Project ID 218454), United States	Quantum-Accurate Multiscale Modeling of Shock Hugoniot, Ramp Compression Paths, Structural and Magnetic Phase Transitions, and Transport Properties in Highly Compressed Metals
2019–2022	Department of Energy, LDRD (Project ID 218319), United States	Accelerating Multiscale Materials Modeling with Machine Learning

2019–2022	Department of Energy, LDRD (Project ID 218456), United States	Improving Predictive Capability in Radiation, Electrical, and High Energy Density Science Simulations with Fast, Accurate, and Consistent Non-Equilibrium Material Properties
2017–2019	Department of Energy, LDRD (Project ID 200202), United States	Making Density Functionals Work for All Materials

Awards & Honours

2023	R&D 100 Award, R&D World, United States
2018	SPOT Award, Sandia National Laboratories, United States
2017	SPOT Award, Sandia National Laboratories, United States
2005	German Academic Exchange Service (DAAD), University of Würzburg, Germany and Rutgers, The State University of New Jersey, United States

Academic Service & Leadership

Institutional Responsibilities

2024–present	Member of Doctoral Advisory Board, Helmholtz-Zentrum Dresden-Rossendorf, Germany
2022–present	Member of Working Group <i>Digitalization</i> , Helmholtz-Zentrum Dresden-Rossendorf, Germany
2021–present	Helmholtz AI Associate, Helmholtz Association, Germany
2022–2024	Member of Working Group <i>Graduate Student Education</i> , Helmholtz-Zentrum Dresden-Rossendorf, Germany
2018	Coordinator of Summer Student Program, Center for Computing Research, Sandia National Laboratories, United States

Reviewing Activities

Research Journals	Nature Communications, Nature Computational Science, Nature Communications Materials, npj Computational Materials, Computer Physics Communications, Scientific Reports, Journal of Chemical Physics, Physical Review Journals, Journal of Physical Chemistry, International Journal of Quantum Chemistry
Funding Agencies	European Research Council (ERC), Swiss National Science Foundation (SNSF), U.S.-Israel Binational Science Foundation (BSF), Pazy Foundation (Israel), Centre Européen de Calcul Atomique et Moléculaire (Switzerland), National High Performance Computing (Germany)

Supervision & Mentoring

Postdocs supervised:

12

PhD students supervised:	5
MSc/BSc students supervised:	17

Teaching Experience

SS 2026	Solid State Physics: Thermal Properties	Lecture, Exercises	TU Dresden, Germany
WS 2025	Atomistic Simulation Methods	Lecture	TU Dresden, Germany
SS 2025	Nanostructured Materials	Lecture, Exercises	TU Dresden, Germany
WS 2024	Atomistic Simulation Methods	Lecture	TU Dresden, Germany

Memberships

German Physical Society (DPG)

Organization of Scientific Meetings and Schools

2024	Critical Use of AI in Quantum Chemistry, Swiss Chemical Society Seminar on Artificial Intelligence 2024, University of Fribourg, Switzerland	Member of Organizing Committee
2023	Accelerating improvements in Density Functional Theory, Swiss Federal Institute of Technology, Lausanne, Switzerland	Organization Committee Chair
2022	Multiscale Modeling of Matter under Extreme Conditions, Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany	Organizing Committee Chair
2022	Strongly Coupled Coulomb Systems, Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany	Local Organizing Committee Chair, Program Committee Member
2022	DFT Methods for Matter under Extreme Conditions, Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany	Organization Committee Chair
2019	Improving the Theory in Density Functional Theory, Swiss Federal Institute of Technology, Lausanne, Switzerland	Organization Committee Chair

2017	Teaching the Theory in Density Functional Theory, Swiss Federal Institute of Technology, Lausanne, Switzerland	Organization Committee Chair
2016	Putting the Theory Back in Density Functional Theory, Institute for Pure and Applied Mathematics, University of California, Los Angeles, United States	Organization Committee Member
2013	Density Functional Theory: Learning from the Past, Looking to the Future, Magnus-Haus of the Deutsche Physikalische Gesellschaft, Berlin, Germany	Organization Committee Member

Publications

Preprints

- 4 K. Ramakrishna, M. Lokamani, **A. Cangj**, "Can MACE Potentials Accurately Describe Magnetism and Phase Stability in Fe-Ni Alloys? A Systematic Benchmark", [arXiv.2605.28395](https://arxiv.org/abs/2605.28395) (2026).
- 3 K. Ramakrishna, M. Lokamani, Z. A. Moldabekov, T. Dornheim, K. Burke, **A. Cangj**, "Thermal PBE in warm dense matter: Does it matter and is it accurate?", [arXiv.2605.25270](https://arxiv.org/abs/2605.25270) (2026).
- 2 Z. Elabid, J. Andrzejewski, B. Brzoza, **A. Cangj**, "Molecules Meet Language: Confound-Aware Representation Learning and Chemical Property Steering in Transformer-VAE Latent Spaces", [arxiv.2605.06303](https://arxiv.org/abs/2605.06303) (2026).
- 1 G. Tejaswini, A. E. Sudheer, A. Kumar, M. Vallinayagam, P. K. Perepu, **A. Cangj**, M. Lokamani, M. Posselt, M. Zschornak, C. Kamal, D. A. Reddy, D. Murali, "Prediction of atomic H adsorption energies in metalloid doped MSSe (M = Mo/W) Janus layers: A combined DFT and machine learning study", [arXiv.2511.16263](https://arxiv.org/abs/2511.16263) (2025).

Research Articles

- 55 K. Shah, **A. Cangj**, "Machine Learning Time Propagators for Time-Dependent Density Functional Theory Simulations", *Mach. Learn.: Sci. Technol.* **7**, 035019 (2026).
- 54 H. Tahmasbi, M. Beerbaum, B. Brzoza, **A. Cangj**, T. D. Kühne, "Scalable Machine Learning Model for Energy Decomposition Analysis in Aqueous Systems", *J. Chem. Phys.* **163**, 214115 (2025).

- 53 **A. Cangj**, L. Fiedler, B. Brzoza, K. Shah, T. J. Callow, D. Kotik, S. Schmerler, M. C. Barry, J. M. Goff, A. Rohskopf, D. J. Vogel, N. A. Modine, A. P. Thompson, S. Rajamanickam, “Materials Learning Algorithms (MALA): Scalable Machine Learning for Electronic Structure Calculations in Large-Scale Atomistic Simulations”, [Comput. Phys. Commun. 314, 109654 \(2025\)](#).
- 52 T. Gawne, Z. A. Moldabekov, O. S. Humphries, K. Appel, C. Baetz, V. Bouffetier, E. Brambrink, **A. Cangj**, C. Crépisson, S. Göde, Z. Konôpková, M. Makita, M. Mishchenko, M. Nakatsutsumi, L. Randolph, S. Schwalbe, J. Vorberger, U. Zastrau, T. Dornheim and T. R. Preston, “Strong geometry dependence of the X-ray Thomson Scattering Spectrum in single crystal silicon”, [Electron. Struct. 7 025002 \(2025\)](#).
- 51 S. Nikolov, K. Ramakrishna, A. Rohskopf, M. Lokamani, J. Tranchida, J. Carpenter, **A. Cangj**, M. A. Wood, “Probing Iron in Earth’s Core With Molecular-Spin Dynamics”, [Proc. Natl. Acad. Sci. U.S.A. 121, e2408897121 \(2024\)](#).
- 50 K. Ramakrishna, M. Lokamani, **A. Cangj**, Electrical Conductivity of Warm Dense Hydrogen from Ohm’s Law and Time-Dependent Density Functional Theory, [Electron. Struct. 6, 045008 \(2024\)](#).
- 49 **A. Cangj**, “Bridging the gap in electronic structure calculations via machine learning”, [Nat. Comput. Sci. 4, 729 \(2024\)](#).
- 48 T. Gawne, H. Bellenbaum, L. B. Fletcher, K. Appel, C. Baetz, V. Bouffetier, E. Brambrink, D. Brown, **A. Cangj**, A. Descamps, S. Göde, N. J. Hartley, M.-L. Herbert, P. Hesselbach, H. Höppner, O. S. Humphries, Z. Konôpková, A. Laso, B. Lindqvist, J. Lütgert, M. J. MacDonald, M. Makita, W. Martin, M. Mishchenko, Z. A. Moldabekov, M. Nakatsutsumi, J.-P. Naedler, P. Neumayer, A. Pelka, C. Qu, L. Randolph, J. Rips, T. Toncian, J. Vorberger, L. Wollenweber, U. Zastrau, D. Kraus, T. R. Preston, T. Dornheim, “Effects of Mosaic Crystal Instrument Functions on X-Ray Thomson Scattering Diagnostics”, [J. Appl. Phys. 136, 105902 \(2024\)](#).
- 47 K. Shah, **A. Cangj**, “Accelerating Electron Dynamics Simulations through Machine Learned Time Propagators”, [ICML Workshop 2024, AI for Science: Scaling in AI for Scientific Discovery, arXiv:2407.09628 \(2024\)](#).
- 46 T. Gawne, Z. A. Moldabekov, O. S. Humphries, K. Appel, C. Bätz, V. Bouffetier, E. Brambrink, **A. Cangj**, S. Göde, Z. Konôpková, M. Makita, M. Mishchenko, M. Nakatsutsumi, K. Ramakrishna, L. Randolph, S. Schwalbe, J. Vorberger, L. Wollenweber, U. Zastrau, T. Dornheim, T. R. Preston, “Ultrahigh resolution x-ray Thomson scattering measurements at the European X-ray Free Electron Laser”, [Phys. Rev. B 109, L241112 \(2024\)](#).
- 45 H. Tahmasbi, K. Ramakrishna, M. Lokamani, **A. Cangj**, “Machine Learning-Driven Structure Prediction for Iron Hydrides”, [Phys. Rev. Mater. 8, 033803 \(2024\)](#).

- 44 V. Martinetto, K. Shah, **A. Cang**, A. Pribram-Jones, "Inverting the Kohn-Sham equations with physics-informed machine learning", *Mach. Learn.: Sci. Technol.* **5** 015050 (2024).
- 43 T. J. Callow, E. Kraiser, **A. Cang**, "Physics-enhanced neural networks for equation-of-state calculations", *Mach. Learn.: Sci. Technol.* **4**, 045055 (2023).
- 42 S. L. S. Balakrishnan, M. Lokamani, K. Ramakrishna, **A. Cang**, D. Murali, M. Posselt, A. A. Sasikala Devi, A. Sharan, "Ab-initio insights on the ultrafast strong-field dynamics of anatase TiO₂", *Phys. Rev. B* **108**, 195149 (2023).
- 41 K. Ramakrishna, M. Lokamani, A. Baczewski, J. Vorberger, **A. Cang**, "Impact of electronic correlations on high-pressure iron: insights from time-dependent density functional theory", *Electron. Struct.* **5**, 045002 (2023).
- 40 L. Fiedler, N. A. Modine, K. D. Miller, **A. Cang**, "Machine learning the electronic structure of matter across temperatures", *Phys. Rev. B* **108**, 125146 (2023).
- 39 S. Kumar, H. Tahmasbi, K. Ramakrishna, M. Lokamani, S. Nikolov, J. Tranchida, M. A. Wood, **A. Cang**, "Transferable Interatomic Potentials for Aluminum from Ambient Conditions to Warm Dense Matter", *Phys. Rev. Research* **5**, 033162 (2023).
- 38 L. Fiedler, N. A. Modine, S. Schmerler, D. J. Vogel, G. A. Popoola, A. P. Thompson, S. Rajamanickam, **A. Cang**, "Predicting electronic structures at any length scale with machine learning", *Npj Comput. Mater.* **9**, 115 (2023).
- 37 T. W. Hentschel, A. Kononov, A. Olmstead, **A. Cang**, A. D. Baczewski, S. B. Hansen, "Improving dynamic collision frequencies: impacts on dynamic structure factors and stopping powers in warm dense matter", *Phys. Plasmas* **30**, 062703 (2023).
- 36 T. Dornheim, M. P. Böhme, D. Chapman, D. Kraus, T. R. Preston, Z. A. Moldabekov, N. Schlünzen, **A. Cang**, T. Döppner, J. Vorberger, "Imaginary-time correlation function thermometry: A new, high-accuracy and model-free temperature analysis technique for x-ray Thomson scattering data", *Phys. Plasmas* **30**, 042707 (2023).
- 35 T. Dornheim, Z. A. Moldabekov, K. Ramakrishna, P. Talias, A. D. Baczewski, D. Kraus, T. R. Preston, D. A. Chapman, M. P. Böhme, T. Döppner, F. Graziani, M. Bonitz, **A. Cang**, J. Vorberger, "Electronic Density Response of Warm Dense Matter", *Phys. Plasmas* **30**, 032705 (2023).
- 34 K. Ramakrishna, M. Lokamani, A. Baczewski, J. Vorberger, **A. Cang**, "Electrical Conductivity of Iron in Earth's Core from Microscopic Ohm's Law", *Phys. Rev. B* **107**, 115131 (2023).
- 33 Z. A. Moldabekov, M. Lokamani, J. Vorberger, **A. Cang**, T. Dornheim, "Non-empirical mixing coefficient for hybrid XC functionals from analysis of the XC kernel", *J. Phys. Chem. Lett.* **14**, 1326 (2023).

- 32 Z. A. Moldabekov, M. Lokamani, J. Vorberger, **A. Cangj**, T. Dornheim, "Assessing the accuracy of hybrid exchange-correlation functionals for the density response of warm dense electrons", *J. Chem. Phys.* **158**, 094105 (2023).
- 31 D. Konar, A. Das Sarma, S. Bhandary, S. Bhattacharyya, **A. Cangj**, V. Aggarwal, "A shallow hybrid classical–quantum spiking feedforward neural network for noise-robust image classification", *Appl. Soft Comput.* **136**, 110099 (2023).
- 30 T. J. Callow, E. Kraisler, **A. Cangj**, "Improved calculations of mean ionization states with an average-atom model", *Phys. Rev. Res.* **5**, 013049 (2023).
- 29 K. Shah, P. Stiller, N. Hoffmann, **A. Cangj**, "Physics-Informed Neural Networks as Solvers for the Time-Dependent Schrödinger Equation", *NeurIPS Workshop Machine Learning and the Physical Sciences*, arxiv:2210.12522 (2022).
- 28 L. Fiedler, N. Hoffmann, P. Mohammed, G. A. Popoola, T. Yovell, V. Oles, J. A. Ellis, S. Rajamanickam, **A. Cangj**, "Training-free hyperparameter optimization of neural networks for electronic structures in matter", *Mach. Learn.: Sci. Technol.* **3**, 045008 (2022).
- 27 L. Fiedler, Z. A. Moldabekov, X. Shao, K. Jiang, T. Dornheim, M. Pavanello, **A. Cangj**, "Accelerating Equilibration in First-Principles Molecular Dynamics with Orbital-Free Density Functional Theory", *Phys. Rev. Res.* **4**, 043033 (2022).
- 26 M. Schörner, B. B. L. Witte, A. D. Baczewski, **A. Cangj**, R. Redmer, "An ab-initio study of shock-compressed copper", *Phys. Rev. B* **106**, 054304 (2022).
- 25 T. J. Callow, D. Kotik, E. Kraisler, **A. Cangj**, "AtoMEC: an open-source average-atom Python code", *Proceedings of the 21st Python in Science Conference*, **37** (2022).
- 24 T. Dornheim, P. Talias, Z. A. Moldabekov, **A. Cangj**, J. Vorberger, "Effective electronic forces and potentials from ab initio path integral Monte Carlo simulations", *J. Chem. Phys.* **156**, 244113 (2022).
- 23 T. J. Callow, E. Kraisler, S. B. Hansen, **A. Cangj**, "First-principles derivation and properties of density-functional average-atom models", *Phys. Rev. Res.* **4**, 023055 (2022).
- 22 L. Fiedler, K. Shah, M. Bussmann, **A. Cangj**, "Deep Dive into Machine Learning Density Functional Theory for Materials Science and Chemistry", *Phys. Rev. Mater.* **6**, 040301 (2022).
- 21 S. Nikolov, J. Tranchida, K. Ramakrishna, M. Lokamani, **A. Cangj**, M. A. Wood, "Dissociating the phononic, magnetic and electronic contributions to thermal conductivity: a computational study in alpha-iron", *J. Mater. Sci.* **57**, 10535 (2022).

- 20 Z. A. Moldabekov, T. Dornheim, G. Gregori, F. Graziani, M. Bonitz, **A. Cangi**,
“Towards a Quantum Fluid Theory of Correlated Many-Fermion Systems from
First Principles”, [SciPost Phys. 12, 062 \(2022\)](#).
- 19 Z. A. Moldabekov, T. Dornheim, J. Vorberger, **A. Cangi**, “Benchmarking
Exchange-Correlation Functionals in the Spin-Polarized Inhomogeneous
Electron Gas under Warm Dense Conditions”, [Phys. Rev. B 105, 035134
\(2022\)](#).
- 18 Z. A. Moldabekov, T. Dornheim, **A. Cangi**, “Thermal Signals from Collective
Electronic Excitations in Inhomogeneous Warm Dense Matter”, [Sci. Rep. 12,
1093 \(2022\)](#).
- 17 Z. A. Moldabekov, Y. K. Aldakul, N. K. Bastykova, S. Sundar, **A. Cangi**,
“Higher harmonics in complex plasmas with alternating screening”, [Phys.
Rev. Res. 3, 043187 \(2021\)](#).
- 16 S. Nikolov, M. A. Wood, **A. Cangi**, J.-B. Maillet, M.-C. Marinica, A. P.
Thompson, M. P. Desjarlais, J. Tranchida, “Data-driven magneto-elastic
predictions with scalable classical spin-lattice dynamics”, [Npj Comput. Mater.
7, 153 \(2021\)](#).
- 15 Z. A. Moldabekov, T. Dornheim, M. Böhme, J. Vorberger, **A. Cangi**, “The
Relevance of Electronic Perturbations in the Warm Dense Electron Gas”, [J.
Chem. Phys. 155, 124116 \(2021\)](#).
- 14 J. A. Ellis, L. Fiedler, G. A. Popoola, N. A. Modine, J. A. Stephens, A. P.
Thompson, **A. Cangi**, S. Rajamanickam, “Accelerating Finite-temperature
Kohn-Sham Density Functional Theory with Deep Neural Networks”, [Phys.
Rev. B 104, 035120 \(2021\)](#).
- 13 T. Dornheim, Z. A. Moldabekov, **A. Cangi**, “A Machine-Learning Surrogate
Model for ab initio Electronic Correlations at Extreme Conditions”, [ICLR 2021
\(2021\)](#).
- 12 K. Ramakrishna, **A. Cangi**, T. Dornheim, J. Vorberger, “First-principles
modeling of plasmons in aluminum under ambient and extreme conditions”,
[Phys. Rev. B 103, 125118 \(2021\)](#).
- 11 T. Dornheim, **A. Cangi**, K. Ramakrishna, M. P. Böhme, S. Tanaka, J.
Vorberger, “Effective static approximation: A fast and reliable tool for warm
dense matter theory”, [Phys. Rev. Lett. 125, 235001 \(2020\)](#).
- 10 T. Baldsiefen, **A. Cangi**, F. G. Eich, E. K. U. Gross, “Exchange-correlation
approximations for reduced-density-matrix-functional theory at finite
temperature: Capturing magnetic phase transitions in the homogeneous
electron gas”, [Phys. Rev. A 96, 062508 \(2017\)](#).
- 9 T. Baldsiefen, **A. Cangi**, E. K. U. Gross, “Reduced-density-matrix-functional
theory at finite temperature: Theoretical foundations”, [Phys. Rev. A 92,
052514 \(2015\)](#).
- 8 **A. Cangi**, A. Pribram-Jones, “Efficient formalism for warm dense matter
simulations”, [Phys. Rev. B 92, 161113\(R\) \(2015\)](#).

- 7 P. Elliott, **A. Cangi**, S. Pittalis, E. K. U. Gross, K. Burke, “Almost exact exchange at almost no computational cost in electronic structure”, [Phys. Rev. A 92, 022513 \(2015\)](#).
- 6 R. F. Ribeiro, D. Lee, **A. Cangi**, P. Elliott, K. Burke, “Corrections to Thomas-Fermi Densities at Turning Points and Beyond”, [Phys. Rev. Lett. 114, 050401 \(2015\)](#).
- 5 H. Mirhosseini, **A. Cangi**, T. Baldsiefen, A. Sanna, C. R. Proetto, E. K. U. Gross, “Virial theorem and exact properties of density functionals for periodic systems”, [Phys. Rev. B 89, 220102\(R\) \(2014\)](#).
- 4 **A. Cangi**, E. K. U. Gross, K. Burke, “Potential functionals versus density functionals”, [Phys. Rev. A 88, 062505 \(2013\)](#).
- 3 **A. Cangi**, D. Lee, P. Elliott, K. Burke, E. K. U. Gross, “Electronic Structure via Potential Functional Approximations”, [Phys. Rev. Lett. 106, 236404 \(2011\)](#).
- 2 **A. Cangi**, D. Lee, P. Elliott, K. Burke, “Leading corrections to local approximations”, [Phys. Rev. B 81, 235128 \(2010\)](#).
- 1 P. Elliott, D. Lee, **A. Cangi**, K. Burke, “Semiclassical Origins of Density Functionals”, [Phys. Rev. Lett. 100, 256406 \(2008\)](#).

Technical Reports

- 7 M. Wood, S. Nikolov, A. Rohskopf, M. P. Desjarlais, **A. Cangi**, J. Tranchida, “Quantum-Accurate Multiscale Modeling of Shock Hugoniot, Ramp Compression Paths, Structural and Magnetic Phase Transitions, and Transport Properties in Highly Compressed Metals”, [Technical Report SAND2022-12792, United States Department of Energy \(2022\)](#).
- 6 S. B. Hansen, A. D. Baczewski, T. Gomez, T. W. Hentschel, C. A. Jennings, A. Kononov, T. Nagayama, K. Adler, **A. Cangi**, K. Cochrane, B. Robinson, A. Schleife, “Improving Predictive Capability in REHEDS Simulations with Fast, Accurate, and Consistent Non-Equilibrium Material Properties”, [Technical Report SAND2022-13455, United States Department of Energy \(2022\)](#).
- 5 N. A. Modine, J. A. Stephens, L. P. Swiler, A. P. Thompson, J. D. Vogel, L. Fiedler, **A. Cangi**, S. Rajamanickam, “Accelerating Multiscale Materials Modeling with Machine Learning”, [Technical Report SAND2022-12875, United States Department of Energy \(2022\)](#).
- 4 J. A. Hubbard, M. A. Omana, D. S. Jensen, **A. Cangi**, T. J. Boyle, “Uranium Aerosol Dynamics: Chemical Kinetics, Primary Particle Formation, Coagulation and Condensation”, Technical Report SAND2019-13154, United States Department of Energy (2019).
- 3 **A. Cangi**, F. Sagredo, E. Decolvenaere, A. E. Mattsson, “Semi-local Density Functional Approximations for Bulk, Surface, and Confinement Physics”, [Technical Report SAND2019-11805, United States Department of Energy \(2019\)](#).

2 **A. Cang**, “An Exchange-Correlation Functional Capturing Bulk, Surface, and Confinement Physics”, [Technical Report SAND2018-7447, United States Department of Energy \(2018\)](#).

1 Author list hidden by publisher, Technical Report SAND2017-13554, United States Department of Energy (2017).

Edited Special Issues and Proceedings

4 J. Yang, **A. Cang**, A. O. Oliynyk, “Machine Learning and Artificial Intelligence in Materials Science and Condensed Matter Physics”, [Materials Today Physics \(2025\)](#).

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