The ThUL School in Actinide Chemistry

19th to 23rd September 2016

Time	Mon (19th)	Tue (20th)	Wed (21st)	Thu (22nd)	Fr (23rd)
8:45	Transfer from hotel	Transfer from hotel	Transfer from hotel	Transfer from hotel	Transfer from hotel
9:15	9:15 **IRE representative** 9:30 **Organizers** 9:45 **M. Patzschke** Computer Codes	**A. Kerridge** Introduction to Active Space	**A. Ikeda-Ohno** XAS Methods	**M. Straka** Theory and NMR (Part 1)	**A. Baranov** Chemical Bonding from Relativistic Methods
10:00	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
10:15	**M. Patzschke** Introduction to Relativistic (Part 1)	**A. Kerridge** RAS-/CAS-SCF Applications	**A. Ikeda-Ohno** XAS Method Applications	**M. Straka** Theory and NMR (Part 2)	**L. Natrajan** Two-Photon-Absorption
11:00	Break	Break	Break	Break	Break
11:15	**M. Patzschke** Introduction to Relativistic (Part 2)	**H. Bahmann** New DFT functionals	**V. Vallet** MD Applications	**B. Schimmelpfennig** Application of Theory to Challenges in Actinide Chemistry	**N. Huittinen** TRLFS in Actinide Sorption and Incorporation
12:00	Lunch	Lunch	Lunch	Lunch	Lunch
13:15	**R. Polly** Theory at Interfaces	**V. Vallet** Molecular Dynamics	*Lab tour in control area*	**M. Trumm** MD Applications	13:00 Bus transfer to DD main station
14:00	Coffee Break	Coffee Break	Social Activity	Coffee Break	
14:15	**M. Patzschke** Point groups	*Exercises:* **ORCA** (MP)	*Mathematisch-Physikalischer Salon*	*Exercises:* **ParaView** – visualizing your results (AB)	
15:00	*Exercises:* **ADF** (MP) 17:00 **Postersession**				
18:00		Transfer back to hotel		Transfer back to hotel	
19:00	Transfer back to hotel			Conference Dinner	

All lectures and exercises will be held at HZDR-IRE, Bautzner Landstrasse 400, D-01328 Dresden, Germany.

Hilke Bahmann

Technische Universität Berlin
Department of Chemistry
Development of DFT functionals, local hybrids

Alexey Baranov

Max Planck Institute for Chemical Physics of Solid
Abteilung Chemische Metallkunde
Chemical bonding in solids, relativistic electron localizability

Atsushi Ikeda-Ohno

Helmholtz-Zentrum Dresden-Rossendorf
Institute of Resource Ecology
X-ray absorption spectroscopy, actinide chemistry

Nina Huittinen

Helmholtz-Zentrum Dresden-Rossendorf
Institute of Resource Ecology
TRLFS, sorption and incorporation, conditioning of nuclear waste

Peter Kaden

Helmholtz-Zentrum Dresden-Rossendorf
Institute of Resource Ecology
NMR of actinides, complexation chemistry of f-elements

Andrew Kerridge

University of Lancaster
Department of Chemistry
Multi-reference calculations for f-elements, treatment of near-degenerate electronic states, spectroscopical data from calculations

Louise Natrajan

The University of Manchester
Radiochermistry
Luminescence and fluorescence spectroscopy, two-photon excitation

Michael Patzschke

Helmholtz-Zentrum Dresden-Rossendorf
Institute of Resource Ecology
Relativistic effects in inorganic chemistry, transition metal complexes, actinides

Robert Polly

Karlsruhe Institute of Technology
Institute of Nuclear Waste Disposal (INE)
Computational surface-molecule interaction

Bernd Schimmelpfennig

Karlsruhe Institute of Technology
Institute of Nuclear Waste Disposal (INE)
Multi-reference calculations with relativistic effects, MD for actinides

Michal Straka

Academy of Sciences of the Czech Republic,
Institute of Organic Chemistry and Biochemistry
Relativistic effects in heavy elements, computational spectroscopy

Michael Trumm

Karlsruhe Institute of Technology
Institute of Nuclear Waste Disposal (INE)
Molecular dynamics for actinides, computational spectroscopy

Valérie Vallet

University of Lille,
Laboratoire de Physique des Lasers, Atomes et Molécules
Electronic structure of heavy elements, spectroscopy, molecular dynamics (MD) for actinides