CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

DFT Methods for Matter under Extreme Conditions

Görlitz, Germany | February 21-22, 2022

Monday

8:45-9:00	Welcome Ronald Redmer, Attila Cangi
9:00-10:00	High-pressure behavior of iron and iron-alloys Gerd Steinle-Neumann
10:00-10:30	Exploring complex chemical composition spaces of planetary ices Andreas Hermann
10:30-11:00	Coffee break
11:00-11:30	From atoms to planets: what can we learn about planetary interiors from ab initio simulations? Francois Soubiran
11:30-11:50	Ab initio simulations for hydrogen-water mixtures Armin Bergermann
11:50-12:10	Metallization of dense fluid helium from ab initio simulations Martin Preising
12:10-14:00	Lunch
14:00-15:00	Stochastic vector computational approaches to finite temperature DFT and electronic structure of large systems Roi Baer
15:00-15:20	Forces from stochastic density functional theory under a nonorthogonal atom-centered basis sets Ben Shpiro
15:20-15:40	Linear weak scalability of density functional theory calculations without imposing electron localization Marcel Fabian
15:40-16:10	Density Functional Theory calculations for high-temperature carbon plasmas Mandy Bethkenhagen
16:10-16:40	Coffee break
16:40-17:10	Ab initio simulations for the ion-ion structure factor of warm dense aluminum Maximilian Schörner
17:10-17:30	Comparisons of density-functional average-atom models and measures of the mean ionization state Timothy Callow
17:30-18:00	Developing Quantum Fluid Theory of Electrons from First Principles Zhandos Moldabekov
18:00-18:20	Summary and discussion 1
18:20-19:45	Poster session
19:45-21:45	Dinner

Tuesday

9:00-10:00	Data-driven and Physics-Informed Modeling of Matter under Extreme Conditions Attila Cangi
10:00-10:20	Hyperparameter optimization for automated DFT surrogate model creation Lenz Fiedler
10:20-10:50	Coffee break
10:50-11:20	Ab initio and machine learning-based simulations of hydrogen in the Earth's core Liang Yuan
11:20-11:50	Learning the exchange-correlation functional from nature with fully differentiable density functional theory Muhammad Kasim
11:50-12:10	Summary and discussion 2
12:10-14:00	Lunch
14:00-14:30	Quantum Monte Carlo Simulation of Warm Dense Matter Tobias Dornheim
14:30-15:00	Trying different xc functionals for warm dense matter Jan Vorberger
15:00-15:30	Towards excitation spectra with the ensemble-generalized DFT approach Eli Kraisler
15:30-16:00	Coffee break
16:00-17:00	Comparing time-dependent DFT and average atom methods in the warm dense regime Andrew Baczewski
17:00-17:30	Electrical Conductivity of Iron in Earth's Core from Microscopic Ohm's Law Kushal Ramakrishna
17:30-18:00	Electronic transport properties of matter under extreme conditions from density functional theory Martin French