

Workshop "Understanding and predicting materials properties by DFT - limits of reliability" and Tutorial FPLO, MPI-CPfS and IFW Dresden, Germany, 07.04.2025 - 11.04.2025

Organizers: Manuel Richter, IFW Dresden
 Ulrike Nitzsche, IFW Dresden
 Klaus Koepernik, IFW Dresden
 Helge Rosner, MPI-CPfS Dresden

Tentative Program, status 13.03.25

Monday, 07.04.2025

IFW

14:00 - 14:50 Registration (IFW, Foyer)

IFW Colloquium (Lecture Hall, coffee is served before in the adjacent atrium)

15:00 "Remain under or leave the academic shelter? Reports of former PhD students and postdocs" with the following contributions:

"Same same but different - flip side perspective" (Deepa Kasinathan, Dresden)

"Do your research" (Carsten Habenicht, Dresden)

"The advantage of things not working straight" (Daniela Heilfort, Ottendorf-Okrilla)

"Welcome to the dark side of life - from Fortran to C# and Java" (Carsten Neise, Dresden)

"Similarities and differences in running a lab and a classroom" (Roman Schuster, Dresden)

16:30 Welcome reception in the IFW atrium

Tuesday, 08.04.2025

MPI-CPfS

09:00 - 09:25 Registration (in front of the seminar room)

09:30 - 09:35 Opening (Helge Rosner)

Chair:	Helge Rosner
09:35 - 10:10	"Bridging scales in materials simulations - quantum versus classical simulations" (Gotthard Seifert, Dresden)
10:10 - 10:45	"Unveiling material dynamics with machine-learned interatomic potentials" (Ferenc Tasnádi, Linköping)
10:45 - 11:05	Coffee
Chair:	Jens Freudenberger
11:05 - 11:40	"Inverse design of materials: From high-throughput workflows to machine learning" (Hongbin Zhang, Darmstadt)
11:40 - 12:15	"The Fe-Si phase diagram, where electrical steel and exoplanets meet" (Stefaan Cottenier, Gent)
12:15 - 12:50	"Strategies for high-throughput optimization of hard magnetic materials" (Ingo Opahle, Darmstadt)

IFW

14:30 - 15:30	Public Lectures "My favorite subject: lectures of two scientific seniors" (seminar room D2E.27)
	"Time series analysis of data sets provided on the COVID-19 dashboard of the RKI: what was the influence of sick certificates by phone in 2020?" (Arnulf Möbius, Dresden)
	"Surprising challenging news and old puzzles from our Old Lady Li_2CuO_2 " (Stefan-Ludwig Drechsler, Dresden)
16:00 - 18:00	Visit to Helmut Eschrig's grave (meeting 16:00 in front of IFW)

Wednesday, 09.04.2025

MPI-CPfS

08:30 - 08:55	Registration (in front of the seminar room)
Chair:	t.b.a.
09:00 - 09:35	"First-principles approach to core-level spectroscopies" (Jan Kuneš, Brno)
09:35 - 10:10	"Simulations of phonon and magnon electron energy loss spectra in scanning transmission electron microscopy" (Jan Ruzs, Uppsala)
10:10 - 10:45	"Modelling low energy ion impacts in 2D materials using DFT simulations" (Silvan Kretschmer, Copenhagen)

10:45 - 11:05	Coffee
Chair:	Oleg Janson
11:05 - 11:50	"Magnetic ground state, electronic structure, and anomalous Hall conductivity of $\text{Cs}_2\text{Co}_3\text{S}_4$: Density-functional calculations" (Madhav P. Ghimire, Kathmandu)
11:40 - 12:15	"Why is PtBi_2 topological?" (Jorge I. Facio, Bariloche)
12:15 - 12:50	"Layer dependence of electronic properties and topological phase transitions in monolayer, bilayer and bulk TaRhTe_4 " (Rajyavardhan Ray, Mesra)

IFW

14:00 - 15:00	Public lecture "Playing with trains and other amusing complex systems", Vito D.P. Servedio, Vienna (Lecture Hall)
15:30 - 18:00	FPLO news and consultations, Klaus Koepernik (room A2E.30)

Thursday, 10.04.2025

MPI-CPfS

Chair:	Ulrike Nitzsche
09:00 - 09:35	"Efficient all-electron hybrid density functionals for atomistic simulations beyond 10,000 Atoms" (Sebastian Kokott, Berlin)
09:35 - 10:10	"Industrial challenges - DFT as a predicting tool" (Samed Halilov, Boston)
10:10 - 10:45	"Understanding AMR in alloys towards better applications" (Wenxu Zhang, Chengdu)
10:45 - 11:05	Coffee
Chair:	Alim Örmeci
11:05 - 11:40	"Self-consistent hybrid functionals: What have we learned so far?" (Daniel Fritsch, Potsdam)
11:40 - 12:15	"Let's talk about solids - Communication between chemists and physicists" (Bertold Rasche, Stuttgart)
12:15 - 12:50	"Bifunctionals" (Kati Finzel, Dresden)

IFW

14:30 - 18:00 FPLO news and consultations, Klaus Koepernik (room A2E.30)

Friday, 11.04.2025

MPI-CPfS

Chair: Ulrich Rößler

09:00 - 09:35 "Altermagnetism in half-antiperovskite-derived structures"
(Harish K. Singh, Salzburg)

09:35 - 10:10 "Design of battery materials assisted by theoretical
simulations and scientific data" (Ruijuan Xiao, Beijing)

10:10 - 10:45 "Transition metal dihalides: from band structure to magnetic
properties" (Alexander Yaresko, Stuttgart)

10:45 - 11:05 Coffee

Chair: Manuel Richter

11:05 - 11:40 "Crystal-field parameters from first-principles and related
applications" (Arthur Ernst, Linz)

11:40 - 12:15 "Electronic structures of kagome metals: kagome or not?"
(Alexander Tsirlin, Leipzig)

12:15 - 12:50 "Ab-initio ligand field theory" (Roland Hayn, Marseille)

12:50 - 13:10 "Topological Hall effect in Fe_3Ga_4 " (Mahdi Afshar, Fairfax VA)

13:10 Concluding remarks (Manuel Richter)
