

	Monday	Tuesday	Wednesday	Thursday	Friday	
8:45 - 9:55		Silke Biermann - <i>Electronic structure calculations using dynamical mean field theory</i>	Ivano Tavernelli - <i>Trajectory-based nonadiabatic dynamics using time-dependent density functional theory</i>	Cecile Hebert - <i>Investigation of molecules at surfaces and chemical reactions by transmission electron microscopy: is a dream becoming true ?</i>		
9:55 - 11:05		Matthieu Verstraete - <i>Ab initio approaches to electron transport</i>	Olle Hellman - <i>Phonons and anharmonics</i>	Andrea Cepellotti – <i>Thermal Transport in 2D Materials</i>	Alec Wodtke - <i>The dynamics of molecular interactions and chemical reactions at metal surfaces: Testing the foundations of theory</i>	
11:05		Coffee break	Coffee break	Coffee break	Coffee break	
11:25 - 12:35		Carsten Baldauf - <i>Molecular dynamics of peptides in isolation and computation on physical observables</i>	Matthias Scheffler - <i>Big-Data Analytics for Materials Science: Concepts, Challenges, and Hype</i>	Markus Elstner - <i>Multiscale simulations of biological structures and processes</i>	Examinations	
12:35		Lunch	Lunch	Lunch	Lunch	
14:15 - 15:25		Tom Rizzo - <i>Biomolecules in isolation – challenges and benchmarks for theory</i>	Christian Carbogno – <i>Thermal Conductivities from First Principles Molecular Dynamics</i>	Group discussion		
15:25		Coffee break	Coffee break			Coffee break
15:50 - 17:00		Matthias Scheffler - <i>Electronic Structure Theory: Introduction and Overview</i>	Michele Ceriotti - <i>Representing and understanding patterns in materials and molecules</i>			Sergey Levchenko – <i>Defects in Solids at realistic conditions</i>
17:00 - 18:10		Claudia Draxl - <i>Beyond density-functional theory: GW and the Bethe-Salpeter equation</i>	Klaus Kern - <i>Molecular nanostructures at surfaces</i>			Karsten Jacobsen - <i>Computational Screening of Light-Absorbing Materials</i>
18:30		Dinner break	Dinner break			Dinner break
20:00 - 21:10	Hardy Gross - <i>Time-dependent density functional theory</i>	poster parade+session	Anatole von Lilienfeld - <i>Machine Learning in Chemical Space</i>			