

Seminar über Theoretische Chemie

jeweils donnerstags, 15:30 Uhr, im Seminarraum 408, 4. OG, Geb. 30.44

- 28.05.20** **Ansgar Pausch**
Isospectrality and symmetry: What graph theory can tell us about chemistry
- 04.06.20** **Xin Gui**
Application of GW-BSE to transition-metal complexes
- 18.06.20** **Jing Liu**
TAPP bulk system with UHF-FDE approach: geometry optimization and property study
- 25.06.20** **Florian Rehak**
Properties of bi- and tetranuclear Cu(I) complexes investigated with GW/BSE within the differential many-body expansion
- 02.07.20** **Patrick Bügel**
Quantum-chemical study of graphene growth on copper
- 16.07.20** **Rodrigo Cortés-Mejía**
Computational study of the electronic properties of 4,4'-bis(carbazol-9-yl)biphenyl (CBP)
- 23.07.20** **Gianni Procida (Institut für Nanotechnologie)**
Ligand binding energies in heteroleptic, dinuclear copper(I) complexes

gez. K. Fink, M.E. Harding, S. Höfener, W. Klopper