

Doktorandenseminar über quantenchemische Methoden zur Beschreibung statischer Korrelationseffekte

Online-Seminar via Zoom, jeweils montags, 10:30 Uhr

- 02.11.20** **Rodrigo Cortés-Mejía**
Static and dynamical correlation: Basic concepts
- 09.11.20** **Patrick Bügel**
The linear variational method: Full configuration interaction (FCI)
- 16.11.20** **Elham Barani**
Multiconfigurational (MCSCF) and complete-active-space self-consistent-field (CASSCF) methods
- 23.11.20** **Jing Liu**
Technical aspects of MCSCF and CASSCF
- 30.11.20** **Marcel Jung**
Density-matrix-renormalization-group technique for CASSCF and FCI
- 07.12.20** **Florian Rehak**
Non-orthogonal configuration interaction
- 14.12.20** **Pascal Förster**
Complete-active-space configuration-interaction density-functional theory (CASCI/DFT)
- 18.01.21** **Ansgar Pausch**
Complete-active-space (CASPT2) and n -electron-valence-state (NEVPT2) second-order perturbation theories
- 25.01.21** **Chengyu Jin**
Multireference configuration interaction (MRCI), difference-dedicated configuration interaction (DDCI), and the multiconfigurational coupled-electron-pair approximation (MCCEPA)
- 01.02.21** **Max Kehry**
Quantum-Monte-Carlo and many-body-expansion FCI methods