Karlsruher Institut für Technologie

Institut für Physikalische Chemie
Abteilung für Theoretische Chemie

Doktorandenseminar über quantenchemische Berechnungen mit TURBOMOLE

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

08.11.21	**Chengyu Jin** Ground-state Hartree–Fock (HF) and DFT computations
15.11.21	**Marcel Lechner** Ground-state MP2, RPA, and coupled-cluster calculations (PNOs, F12)
22.11.21	**Elham Barani** Molecular properties, wave function analysis, visualization
29.11.21	**Florian Rehak** Parallel computing, memory and scratch-space management
06.12.21	**Rodrigo Cortés-Mejía** Reaction pathways and transition state optimization
13.12.21	**Pascal Förster** Treatment of open-shell systems (UHF, ROHF, broken symmetry, SOCI)
20.12.21	**Marius Rabung** Treatment of excited states (TDDFT, CC2, two-photon absorption)
10.01.21	**Jing Liu** Embedding and solvation effects
17.01.21	**Ansgar Pausch** Two-component calculations (relativistic effects, external magnetic field)
24.01.22	**Patrick Bügel** Periodic boundary conditions
31.01.22	**Max Kehry** *GW* approximation and Bethe–Salpeter equation

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