

Special Topics in Theoretical Chemistry

Reiher Group Seminar // Spring Semester 2015

Name	Date	Title
Jochen Autschbach ^a	Feb. 10	Calculating Magnetic Properties of Open-Shell Metal Complexes [<i>guest talk</i>]
Stefan Knecht ^b	Feb. 17	The Electron Correlation Problem in the Lower Part of the Periodic Table
Pascal de Buren	Feb. 24	Constructing the Jacket Potential for Small Molecular Systems on a DFT Grid [<i>semester project</i>]
Florian Krausbeck	Mar. 10	Conditional Molecular Scaffold Design
Alain Vaucher	Mar. 17	Self-Consistent Semi-Empirical Methods for Real-Time Quantum Chemistry [<i>master thesis</i>]
Arseny Kovyrshin	Mar. 24	Tensor Network Parametrization
Sebastian Keller	Mar. 31	MAQUIS::DMRG::SU2::2site-opt
Stefano Battaglia	Apr. 21	Implementation of the Relativistic (Four-Component) DMRG Approach in Maquis [<i>master thesis</i>]
Boris Le Guennic ^c	Apr. 28	Molecular Magnetism of Lanthanide-Based Complexes: Ab initio Considerations [<i>guest talk</i>]
Yingjin Ma	May 5	The Second Derivatives of a MPS-Based DMRG-SCF State
Danil Kaliakin ^d	May 12	Modeling Intersystem Crossing in Metal–Sulfur Proteins [<i>guest talk</i>]
Kristine Pierloot ^e	May 19	Spin-State Energetics in First-Row Transition Metal Complexes: Role of 3s3p Correlation [<i>guest talk</i>]
Joachim Ballmann ^f	July 11	Synthesis and Reactivity of Trisamidophosphine Complexes [<i>guest talk</i>]
Cherif F. Matta ^g	Aug. 5	Electron Localization–Delocalization Matrices: Some Recent Applications [<i>guest talk</i>]

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