Karlsruher Institut für Technologie

Institut für Physikalische Chemie
Abteilung für Theoretische Chemie

Seminar über Theoretische Chemie

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

24.04.14 **Dr. Tomáš Kubař**
Multi-scale simulation of biological electron transfer

08.05.14 **PD Dr. Artur Böttcher**
Non-IPR fullerenes as building blocks for monodisperse nanomaterials

15.05.14 **Nils Middendorf**
Analytic nuclear gradients for the quasi-relativistic X2C approach

23.05.14[*)] **Monika Borkowska-Panek**
Surfaces of iron oxides and their interactions with peptides: theoretical studies

05.06.14 **Dr. Lies Broeckaert (Uni Marburg)**
Studies on heterometallic polyanions with a modified genetic algorithm

12.06.14[**)] **Anna Hehn**
Explicitly correlated random phase approximation

26.06.14 **Katharina Krause**
2c-CC2: a coupled-cluster based approach to spin-orbit effects in excited states

03.07.14 **Michael Kühn**
Two-component methods in the framework of time-dependent density-functional theory

10.07.14 **JProf. Dr. Tobias Schwabe (Uni Hamburg)**
The polarizable embedding method in the coupled-cluster framework

gez. W. Klopper

*) Freitag! Seminarraum AOC 401, Geb. 30.45
**) Seminarraum AOC 301, Geb. 30.45