IAP Seminar

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Tuesday, 5th December 2017, 16:00 s.t.

TU Wien, Institut für Angewandte Physik, E134
1040 Wien, Wiedner Hauptstraße 8-10
Yellow Tower „B“, 5th floor, SEM.R. DB gelb 05 B

Calculating ground and excited state properties of solids & surfaces using beyond-DFT ab-initio methods

This presentation will review recent progress in applying periodic coupled cluster theories to the study of surfaces and solids. We will briefly discuss methods that reduce the computational cost and accelerate convergence of calculated properties towards the complete basis set as well as thermodynamic limit [1-4]. These recent developments have enabled an increasing number of ab-initio studies and allowed for assessing the accuracy of coupled cluster theories by comparing to experimental findings as well as quantum Monte Carlo results. The presented applications will include phase transitions of solids [5], molecular adsorption energies [6-7], hydrogen dissociation on silicon surfaces as well as ground and excited state studies of defects in solids.

1. A. Grüneis, Phys. Rev. Lett. 115 066402 (2015).
2. G. H. Booth, T. Tsatsoulis, G.K.L. Chan, A. Grüneis, J. Chem. Phys. 145 084111 (2016).
3. K. Liao, A. Grüneis, J. Chem. Phys. 145 141102 (2016).
4. F. Hummel, T. Tsatsoulis, A. Grüneis, J. Chem. Phys. 146 124105 (2017).
5. A. Grüneis, J. Chem. Phys. 143, 102817 (2015).
6. T. Tsatsoulis, et al. , J. Chem. Phys. 146 204108 (2017).
7. Y. S. Al-Hamdani, et al., J. Chem. Phys. 147, 044710 (2017).

All interested colleagues are welcome to this seminar lecture (45 min. presentation followed by discussion)

Friedrich Aumayr
(LVA-Leiter)

Ulrike Diebold
(Seminar Chair)