Julius-Maximilians-
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WÜRZBURG

Kolloquium der Physikalischen und Theoretischen Chemie

Dienstag, 04.07.2017 **Hörsaal D, Chemiezentralgebäude, 17:15 Uhr**

Sprecher: Ralf Tonner

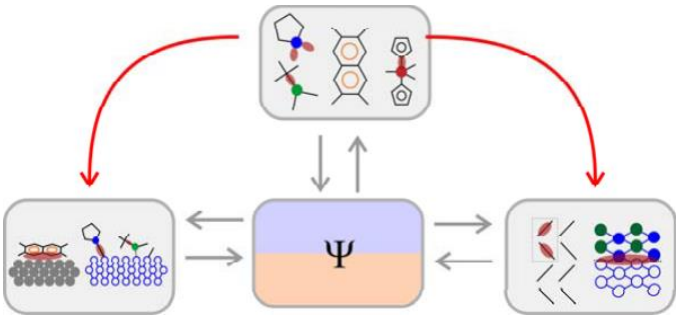
(Universität Marburg)

Titel: Computational chemistry for functional materials

Abstract:

In molecular chemistry, quantum chemical methods reached a state where accuracy is comparable or even exceeds experimental approaches. Similarly, bonding and reactivity concepts based on various analysis methods are well established and very often complement experimental studies to aid interpretation or predict new chemistry. Surprisingly, this fruitful interplay of quantitative and qualitative theoretical approaches and experiment has barely been extended to surface and material sciences.[1]

Our work deals with the application of computational chemistry methods, mostly dispersion-corrected density functional theory, to material sciences questions. Thereby we focus on the transfer of bonding and reactivity concepts from molecular chemistry to surfaces and solids.
Specifically, with the aid of a periodic extension of the energy decomposition analysis (pEDA) method giving chemical insight based on well-defined interaction terms.[2]
Application of the concept toward organic functionalization of semiconductor surfaces[3], metalorganic interfaces[4], semiconductor hetero-interfaces[5] and thin-film deposition processes[6] will be shown.



Electronic structure theory and bonding analysis as the “engine“ for the transfer of concepts from molecular to extended systems.

[1] a) A. Nilsson, L. G. M. Pettersson, J. Nørskov, Chemical Bonding at Surfaces and Interfaces, Elsevier, Amsterdam, 2007; b) R. Hoffmann, Solids and surfaces, VCH, New York, Weinheim, 1988.
[2] M. Raupach, R. Tonner, J. Chem. Phys. 2015, 142, 194105.
[3] a) J. Pecher, R. Tonner, ChemPhysChem 2017, 1, 34; b) J. Pecher, G. Mette, M. Dürr, R. Tonner, ChemPhysChem 2017, 18, 357; c) J. Pecher, C. Schober, R. Tonner, Chem. – Eur. J. 2017, 23, 5459.
[4] P. Rosenow, P. Jakob, R. Tonner, J. Phys. Chem. Lett. 2016, 7, 1422.
[5] A. Beyer, A. Stegmüller, K. Volz, R. Tonner et al. Chem. Mat. 2016, 28, 3265.
[6] a) A. Stegmüller, M. Dürr, K. Volz, R. Tonner et al., Chem.--Eur. J. 2016, 22, 14920; b) P. Rosenow, R. Tonner, J. Chem. Phys. 2016, 144, 204706; c) A. Stegmüller, R. Tonner, Chem. Vap. Depos. 2015, 21, 161.

Organisation: V. Engel

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