

WELCOME TO THE COMPUTATIONAL MATERIALS SCIENCE SEMINAR

CHEMICAL BONDING, LOBSTER, AND ALL THAT



ABSTRACT

Population analysis has held a prominent place in quantum chemistry for decades already. Likewise, periodic bonding indicators such as COOP (introduced in 1983) and its DFT equivalent COHP (from 1993) have been helpful, the latter carried out using local-basis codes such as TB-LMTO-ASA. COHP analysis has allowed to chemically understand three-dimensional Peierls distortions, spin polarization in itinerant magnets, stoichiometries of phase-change materials, and a lot more. While plane-wave packages such as VASP, ABINIT, Quantum ESPRESSO etc. offer computational advantages compared to LMTO, they lack locality, so the aforementioned chemical concepts were unavailable. Nonetheless, the local COHP information can be analytically reconstructed by transferring PAWs to localized bases built from contracted STOs, as implemented in the LOBSTER code (www.cohp.de). In addition, the generalized DOE function (density-of-energy, yielding the band-structure energy when integrated up to the Fermi energy) is ready to go, and it nicely serves as the energy fingerprint of any kind of material.



Speaker: Richard Dronskowski

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BIOGRAPHY

Richard Dronskowski was born in Brilon, Germany, in 1961, and he studied chemistry and physics at the University of Münster in the early 1980s. After receiving his diplomas in 1987 and 1989, he got his Ph. D. (Dr. rer. nat., to be precise) in 1990 from the Technical University of Stuttgart and the (neighboring) Max Planck Institute for Solid State Research; the thesis was entitled "Condensed Clusters in Oxides and Arsenides of Molybdenum". Five years later, he received both habilitation and venia legendi from the University of Dortmund. Boy, those were the good old days!

In his professional career he worked as a visiting scientist at Cornell University and at the above-mentioned Max Planck Institute at Stuttgart. In 1997 he took the Chair of Inorganic and Analytical Chemistry and became Director of the Institute of Inorganic Chemistry at RWTH Aachen University. In 2006 this chair was eventually given a new name (see above) to better reflect the particular research that is being done at this group.

LOOKING FORWARD TO SEEING YOU!