O 81: Poster Session - New Methods: Theory

Time: Wednesday 18:15–20:00   Location: P2/EG

O 81.1   Wed 18:15   P2/EG

Specular-diffusive decomposition of the transmission function — Michael Czerner[1,2], Jonas F. Schäfer-Richarz[1,2], and •Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Zentrum für Materialforschung (LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

A conscious design of electronic transport is crucial for all nanoelectronic devices. This necessitates a precise understanding of the behaviour of electrons as they traverse a device. To this end, $k_\parallel$-resolved transmission maps provide a valuable tool for relating the observed phenomena, such as tunnel magnetoresistance effects, to microscopic processes. A description by slabs of material with a 1×1-supercell is insufficient when imperfections within the device are to be described. Impurities, dislocations, skyrmions, and thermal disorder may modulate the transport properties of a nanoelectronic device. In essence, such imperfections break translational invariance. Because most such defects are localized, the transmission can be projected onto the perfectly ordered leads of the transport system. Thus, a transmission map $T(k_\parallel, k'_\parallel)$ connecting Bloch states in the left and right lead can be recovered. This transmission map may be split into a specular part, which is $k_\parallel$ conserving, and a diffusive part, which allows scattering between $k_\parallel$-vectors of the leads. We implemented this decomposition of transmission maps in our Korringa-Kohn-Rostoker code. As a test case, we show the transmission through iron bulk, where either atomic positions or their magnetic moments were randomly displaced.

O 81.2   Wed 18:15   P2/EG

PyFLOSIC: Insights, developments and progress — •Sebastian Schwalbe[1], Jakob Kraus[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Germany — [2]Central Michigan University, USA

We present the current status as well as new developments within PyFLOSIC [1,2], an Open-Source implementation of the Fermi-Löwdin orbital self-interaction correction (FLO-SIC) [3,4] based on the highly modular and modern PySCF code infrastructure. FLO-SIC aims to counter the well-known self-interaction error (SIE) of density functional theory (DFT). Within PyFLOSIC, the FLO-SIC method can be applied to any functional implemented in the libxc library. The new implementation is written in the python programming language. The choice of python enables fast developments to implement numerical speed-ups, algorithmic advances as well as the extension of the FLO-SIC method to new research topics. Various results for extended molecules and preliminary results for solids are discussed in detail.

[1] S. Schwalbe et al., arXiv:1905.02631 (2019)
[2] S. Schwalbe et al., JCC, vol. 40, 2843 (2019)
[3] S. Schwalbe et al., JCC, vol. 39, 2463 (2018)
[4] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)

O 81.3   Wed 18:15   P2/EG

Fermi-orbital descriptors: Interpretation, generation and bond order — •Sebastian Schwalbe[1], Jakob Kraus[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Germany — [2]Central Michigan University, USA

Fermi-orbital descriptors (FODs) [1,2] are the core elements of the Fermi-Löwdin orbital self-interaction correction (FLO-SIC) method [3,4]. We provide an interpretation of these FODs and suggest that they carry chemical bonding information. A central result is that optimized FOD positions forming an electronic geometry are in correspondence with conceptional expectations from Linnett's double-quartet theory, an extension of Lewis' theory of bonding. In addition, the implementation and application of independent methods for the automatic generation of these chemically important descriptors are discussed.

[1] S. Schwalbe et al., JCC, vol. 40, 2843 (2019)
[2] S. Schwalbe et al., arXiv:1905.02631 (2019)
[3] S. Schwalbe et al., JCC, vol. 39, 2463 (2018)
[4] M. R. Pederson et al., JCP, vol. 140, 121103 (2014)