Partially Occupied Wannier Functions and Quantum Transport in Nano-Scale Contacts

K. S. Thygesen

Center for Atomic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

I will present a method for constructing maximally localized Wannier functions (WFs) for general systems including non-periodic metallic systems such as molecules adsorbed on a metal surface or a molecule attached between metallic electrodes. The resulting partially occupied WFs [1] have improved symmetry and localization properties as compared to the WFs constructed from the occupied subspace. In the second part I discuss how the partially occupied WFs can be used to calculate the Landauer-Büttiker conductance of nano-scale contacts with plane-wave accuracy within a DFT framework [2]. As an application of the WF-transport scheme it is demonstrated how the presence of impurity gas atoms can affect the electrical properties of Ag and Au monatomic chains. Finally, it is shown how the minimal WF basis can be combined with the GW approximation to address correlation effects in quantum transport through realistic nano-scale contacts [3].

[1] K. S. Thygesen, L. B. Hansen, and K. W. Jacobsen, Phys. Rev. Lett. **94**, 026405 (2005).

[2] K. S. Thygesen and K. W. Jacobsen, Chem. Phys. **319**, 111 (2005).

[3] K. S. Thygesen and A. Rubio, J. Chem. Phys. **126**, 091101 (2007).