

Title: Novel strategies for the evaluation of the electron and thermal transport in nanostructures

Abstract: The study of quantum transport in nanostructures requires the development of simulation tools able to address the complexity of the structures at the atomistic level and the intrinsic quantum mechanical effects. Here, we present an integrated method – implemented in the WanT package [1] – to treat both electron and thermal transport at the nanoscale, at the same level of accuracy. The core methodology combines state-of-the-art DFT (and beyond), plane-wave, pseudopotentials calculations with a real-space Green's functions method based on an extended Landauer formalism to describe quantum conductance.

Advanced projections techniques [2] are implemented to characterize the electronic structure in the real space, while a unified finite-fields/finite-differences approach is proposed to evaluate the vibrational properties [3,4] that enter in Landauer formulation. This approach allows us to directly link the transport properties of a device (e.g. interface resistance, heat stability and dissipation) to the chemical coupling, dimensionality, and atomistic structure of the system. Once the electron and thermal conductivities are known, thermoelectric ZT figure of merit can also be obtained [5]. Electronic (e.g. self-consistent Hubbard U, Fermi surfaces, etc) [2,6] and dielectric properties (e.g. Born charges, dielectric tensor) as well as vibrational spectroscopies (IR and Raman) [4] can be easily obtained, as byproduct of the present method.

Here, we present a comprehensive first-principles study of the electron and thermal transport properties of a few paradigmatic low-dimensional nanostructures, namely (i) graphene/dielectric interfaces [7] and (ii) metal-doped TCO nanowires [8]. These systems have been widely investigated for their potential application in optoelectronic, photovoltaics and thermoelectric devices.

References:

- [1] A. Calzolari, N. Marzari, I. Souza and M. Buongiorno Nardelli, Phys. Rev. B 69, 035108 (2004) WanT – www.wannier-transport.org.
- [2] L. A. Agapito, A. Ferretti, A. Calzolari, S. Curtarolo, and M. Buongiorno Nardelli, Phys. Rev. B 88, 165127 (2013).
- [3] A. Calzolari, T. Jayasekera, K.W. Kim, and M. Buongiorno Nardelli, J. Phys. Cond. Matter. 24, 492204 (2012).
- [4] A. Calzolari and M. Buongiorno Nardelli, Sci. Rep. 3 2999 (2013).
- [5] Y. Chen, T. Jayasekera, A. Calzolari, K.W. Kim, and M. Buongiorno Nardelli, J. Phys.: Condens. Matter 22, 372202 (2010).
- [6] L. Agapito et al., preprint (2014).
- [7] R. Mao, B. D. Kong, K. W. Kim, T. Jayasekera, A. Calzolari, and M. Buongiorno Nardelli, Appl. Phys. Lett. 101, 113111 (2012).
- [8] A. Calzolari et al. preprint (2014).