

Wannier Functions and Quantum Transport in Nanostructures

Marco Buongiorno Nardelli

*Department of Physics, North Carolina State University, Raleigh, NC 27695- 8202,
U.S.A. and Computational Science and Mathematics Division, Oak Ridge National
Laboratory, Oak Ridge, TN 37830, U.S.A.*

Determining the quantum ballistic conductance of a nanosystem has become of primary interest in recent years for the promise of novel technological applications for nanoscale quantum electronic devices. In particular, on the theoretical side, a fully first principle theory of electronic transport is highly desirable. In this talk, I will discuss how the use of Maximally-Localized Wannier functions has led to important advances in the development of efficient techniques to compute quantum conductance from first principles [1] and show examples of prototypical applications, ranging from molecular devices and carbon nanotubes systems to ferroelectric tunnel junctions.

[1] WanT project, <http://www.wannier-transport.org>