Ab initio modeling of quantum transport at the nanoscale

Vincent Meunier

Rensselaer Polytechnic Institute, 110 8th Street, Troy, NY 12180, USA
meuniv@rpi.edu

Abstract

The unification of scalable mathematical algorithms, novel electronic structure methods, and advanced computing tools have enabled the development of predictive tools for the discovery of novel phenomena and principles for the design of new molecular electronics with breakthrough properties. Theoretical methods have now evolved to a point where the properties of materials can be successfully predicted based solely on their atomic structure and with limited or no experimental input. Therefore, computational sciences capabilities can substantially speed up the search for novel materials and devices, especially when theoretical work proceeds in parallel and in collaboration with strong experimental efforts.

Here we will present findings from a number of our research endeavors dedicated to various aspects of nanoscale and molecular electronics. We will focus on both two- and multi- terminal setups. First, we will show how the position of a single embedded molecule can be modified to change the overall conduction state of a nanowire [1, 2]. The presentation will proceed with a specific example of the key role played by interface states in the coupling between electrodes and molecules for DNA sequencing [3]. Further examples of two-terminal applications will be shown for the case of low dimensional carbon-based structures, including an investigation of the role of structural and chemical defects [4, 5], and the role of nano/macro interfaces [6]. Turning to multi-terminal systems, we will show how one-dimensional structures can be chemically combined to create complex networks with emerging properties, such as rectification [7] and addressability [8]. We will also present a recently developed technique where first-principles calculations can be mapped onto an open-system setup for multi-terminal transport calculations [9], and show how this technique is employed to predict unusual electronic behavior in a system comprised of a molecule embedded between three terminals[10].

The presentation will conclude with a discussion of a number of possible future directions where atomic scale calculations can be used to enhance our understanding of electronic transport in low-dimensional structures.

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