

Multiscale Simulations and Design of Nano Devices and Materials

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Nanoscale electronics promises to dramatically enhance computing, sensing, and harvesting of solar energy. However, molecular-scale control and manufacturing are difficult tasks, which require major advances to become practical in large-scale applications. The development of molecular-scale devices and circuits can be greatly enhanced by predictive simulation of their components and by formulating design principles that will make nanoscale circuitry smaller, more efficient and more reliable. I will discuss the results of several recent investigations of electron transport in devices based on organic molecules, and of defects and doping in graphene nanoribbons.

For molecules sandwiched by metallic¹ or semiconductor leads^{2, 3}, the transport properties are calculated using real-space multigrid method within density functional theory and non-equilibrium Green function formalism. Mechanism of the negative differential resistance is revealed by analyzing the position dependent density of states under different bias. It is found that the alignment of the individual molecular states, HOMO and/or LUMO, with the Fermi level of the leads plays an important role in determining the I-V characteristics of the single molecular devices. Current-induced high and low conductance switching in molecular devices is investigated by calculating the atomic forces under bias and relaxing the atomic positions accordingly.

In contrast to conventional two-terminal setup, the organic molecules connected to multiple electrodes exhibits interesting new properties, such as pronounced negative differential resistance as pseudo-gating effect. General trends and potential applications for multi-terminal systems are demonstrated.

Electronic, magnetic, and optical properties of carbon nanoribbons, a new material for nano scale electronics, are also investigated within DFT⁴. Our simulations show that the defects at the edges, such as roughness of the edge and/or substitution atom doping, will destroy the spin polarization and lead to a non-magnetic ground state. The interplay of impurity and edge states in zigzag ribbons leads to rich electronic effects, resulting in semiconducting or metallic behavior depending on the dopant position.

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