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Resonant Tunneling into p-Stacked Molecular Wires

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One promising approach to assemble molecules into an active electronic component involves self-assembling monolayer (SAM) techniques. This would ideally lead to the formation of highly packed and organized molecular structures on a metallic template. Once a dense structure is formed, molecular interactions should become significant. We have studied the influence of π-orbital coupling in arenes-based assembly on its resulting electronic and electrical properties. The conduction and the field-switching properties of the assembly are compared as the intermolecular distances are reduced to below 5 Å. We have investigated the electron transport within a single molecule, and more importantly, between the molecules which form a 1D molecular wire. We have also explored different electrode geometries. For specific electrodes arrangement, we predict a large conductance modulation upon application of a transverse gate field, for which the switching mechanism involves a delocalized π-resonance - i.e. resonant tunneling in the intermolecular π- and π*-bands of the molecular assembly.

Alain Rochefort has a broad expertise in experimental and theoretical physical chemistry: B.Sc. Chemistry (UdeM, 1987), M.Sc. Quantum Chemistry (UdeM, 1989), Ph. D. Heterogenous Catalysis (Paris VI, 1992), and post-doctoral surface science studies at Institut de Recherche sur la Catalyse (Lyon), at Université Laval (Québec), and at INRS-Énergie et Matériaux (Varennes). He is the project leader of the Nanostructure group at the Centre de recherche en calcul appliqué (CERCA) since 1997, where he has made significant theoretical contributions, and more especially in the field of carbon nanotubes. He has jointed the Engineering Physics Department at École Polytechnique de Montréal in 2002 as an assistant professor. His present research in computational nanoscience focuses on the fundamental properties of assembled molecular systems, and includes electronic structures, electron transport, and interface properties, as well as the modeling of nanostructure growth and STM imaging.