Dangling-bond wires on H-passivated Si(001) as surface interconnects

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Résumé

The development of molecular electronics strongly relies in our ability to individually connect single atoms and molecules. Unfortunately, the development of working devices is being deterred by the lack of low- resistivity leads and interconnects of the same size scale as the active atomic device. Promising breakthroughs in silicon-based interconnects have been the creation of many types of silicon nanowires. An alternative but related approach has been proposed in which surface electronic states were engineered, taking advantage of the very local nature of silicon bonds. By using the tip of a scanning tunneling microscope (STM) to create dangling-bond nanowires on silicon surfaces, surface electronic states can be precisely tuned.
In this work we propose to explore the structural and electronic properties of such wires thanks to the use of (i) DFT-based calculations, and (ii) Near-Equilibrium Green's Function theory to simulate the transport properties.
In addition to a rationalization of electronic transport in these systems, we propose a strategy to enhance not only charge transport but also spin transport in dangling-bond wires. Finally, we address the critical issue of leakage current, i.e. the loss of surface current due to a leak in the bulk silicon motivated by the presence of dopants.

Mots-Clés: electronic transport, DFT, NEGF, spintronics, surface

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