Realistic multi-terminal first-principles transport simulations of two-probe STM measurements on Ge(001) surface: demonstration of quasi-ballistic transport through dangling-bond dimer wires

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The ability to fabricate high-quality dangling-bond (DB) dimer wires on Ge(001):H was demonstrated and their transport properties were measured with atomic level precision using a two-probe Scanning Tunneling Microscope (STM) setup [1]. Moreover, DB-dimer wires on both Si and Ge(001):H substrates were predicted to be robust against electron doping and capable of sustaining ballistic transport [2]. Given the complexity of such experiments and the largely unexplored character of the multi-probe technique, where more than one STM tip approach simultaneously the system under analysis, theoretical support is crucial to help the interpretation and understanding of observations.

We present a joint theoretical and experimental study of the transport through DB-dimer wires on bare Ge(001) surfaces, with more emphasis on the theoretical aspects. Realistic first-principles calculations using Density Functional Theory together with Non-Equilibrium Greens Function formalism [3,4] of a four-terminal setup involving up to 5000 atoms were carried out to simulate the two-tip experiment on the semiconductor surface. Comparison of both experimental and theoretical results confirm a quasi-ballistic coherent electronic transport through unoccupied states of Ge dimer-row wires on the surface. Our results indicate the possibility to use Ge(001) dimer rows as interconnects for atomic-scale devices fabricated on these surfaces.

[1] M. Kolmer et al. *J. Phys.: Cond. Mat.* **29**, 444004 (2017).
[2] M. Engelund et al. *J. of Phys. Chem. C* **120**, 20303 (2016).
[3] E. Artacho et al. *Phys. Stat. Sol. (b)* **215**, 809 (1999). J. M. Soler et al. *J. Phys.: Cond. Mat.* **14**, 2745 (2002).
[4] M. Brandbyge et al. *Phys. Rev. B* **65**, 165401 (2002). N. Papior et al. *Comp. Phys. Comm.* **212**, 8 (2017).