# DENSITY FUNCTIONAL THEORY INVESTIGATION OF RARE EARTH SILICIDE NANOWIRES

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Quasi one-dimensional electron systems are of both fundamental interest because of their unusual physical properties as well as potentially interesting for devices on the nanometer scale. In this respect, rare earth (RE) silicide nanowires on silicon (001)-surfaces are of special interest, because the RE silicides exhibit useful physical properties such as low Schottky-barriers, thermal stability and low electrical resistivity one the one hand, and because the silicon (001)-surface is well known and very common in today's technology on the other.

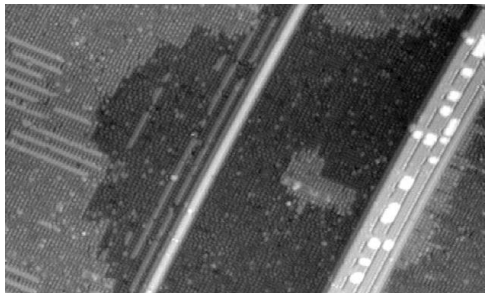

Fig. 1: STM image "showing two broad nanowires at the center and the right of the image as well as some remaining thin nanowires on the left" [1]

One special feature of the RE silicide nanowires is their preparation, as they grow self-organized controlled by macroscopic parameters such as temperature, deposition amount, and atomic number of the RE. Under variation of these parameters, different systems of RE silicide nanowires have been studied experimentally [1].

Unfortunately, the exact knowledge of their atomic structure, which is crucial for understanding their physical properties, is still incomplete. As a first step towards understanding the nanowires structural and their electronic properties, we have investigated different wire models from first-principles within density functional theory (DFT). Thereby erbium is chosen as prototypical trivalent rare earth ion and its 4f-electrons are treated as frozen state in the atomic core.

The wire models base all on the hexagonal RE silicide structure suggested from the experiment [1]. They have been categorized corresponding to three degrees of freedom, namely width, height and depth of burial. After comparing the formation energy of different models within ab-initio thermodynamics, electronic band structures and densities of states are calculated for the stable wires. Structural and electronic properties are discussed and compared with available STM[1], STS[2] and ARPES[1] measurements.

*Keywords:* nanowires, rare earth, silicide, DFT

**References**

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[2] I. Miccoli, F. Edler, H. Pfnür, S. Appelfeller, M. Dähne, K. Holtgrewe, S. Sanna, W. G. Schmidt, C. Tegenkamp, Phys. Rev. B 93 (2016) 125412.