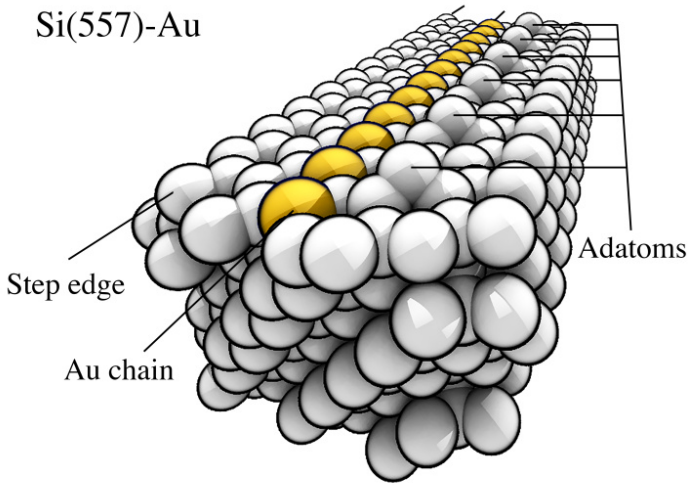
Hessisches Kompetenzzentrum für Hochleistungsrechnen

Ground- and Excited-State Properties of Substrate-Supported Nanowires Calculated From First Principles



Introduction

Ideal one-dimensional electronic systems are characterized by unusual and fascinating physical phenomena, including quantization of conductance, charge-density waves, Luttinger liquid behavior, as well as a variety of instabilities associated with a wealth of phase transitions. Real one-dimensional electronic systems are typically realized as substrate supported atomic wires, and thus inevitably coupled in two (2D) or three (3D) dimensions.

While the coupling with higher dimension affects the 1D properties, it might be employed to control and manipulate the physical properties of the atomic wires. The goal of this project is to understand the intertwinement between the properties of the 1D systems and their environment.

Methods

Our main tool for atomistic modelling is the software package VASP (Vienna Ab initio Simulation Package) It is a computer program for first principles atomic scale materials modelling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics. VASP makes use of efficient iterative matrix diagonalisation techniques, like the residual minimisation method with direct inversion of the iterative subspace (RMM-DIIS) or blocked Davidson algorithms to determine the electronic

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groundstate of the investigated systems. Highly customizable parallelization schemes are implemented in VASP. In particular, parallelization (and data distribution) over bands, parallelization (and data distribution) over plane wave coefficients, as well as parallelization over k-points (no data distribution) can be used at the same time on massively parallel systems in order to obtain high computational efficiency.

Results

Au wires grown on vicinal Si(111) surfaces are an ideal playground to test the coupling of the atomic chains with higher dimensions, as the miscut angle (i.e. the deviation from the ideal Si(111) surface) controls the wire width (single or double atomic rows) and the interwire distance. We have modelled both the groundstate and excited state properties of different vicinal structures, in particular Si(557)-Au (see Fig. 1) and Si(553)-Au. In a further step, we have explored the possibility to tune the wire conductivity by adsorption of foreign species. Adsorption of H and O is found to affect differently single and double Au wires [1]. The coupling of the wires to higher dimensions through the substrate results in the breakdown of the nearly-free electron gas model [2-4]. Thus, the wires are more appropriately described as extremely anisotropic 2D objects than as purely 1D.

Discussion

Besides exploring different 1D-Systems and the tuning of their properties, we plan to develop and implement first-principle methods for the investigation of their spectroscopic properties. Similarly to the computational approach we employed to model Raman-Spectroscopy of surface structures [5], we are currently developing computational methods for the simulation of RAS spectroscopy.

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