Ab initio (from the electronic structure) calculations of processes in materials and (bio)molecules.

ABSTRACT BOOK
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Ground state structures of neutral and charged clusters

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The global minima structures of charged and neutral clusters were investigated in numerous studies during the last few decades. Whereas neutral clusters are at the focus of most theoretical work, charged cluster are nearly exclusively studied in experiment. The important relation between the charged and neutral minima was however not studied in much detail. We provide a closer look at the global and first few local minima of small and medium sized charged and neutral Si and Mg system within density functional theory. For silicon clusters, we find that in all cases in the range 8–19 atoms, the neutral and charged global minima structures are different. For Mg system we find the same result for 3–19 atoms.

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Unbiased determination of structural and electronic properties of gold clusters with up to 58 atoms

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Isolated neutral AuN clusters are studied using a parametrized density-functional tight-binding method combined with genetic algorithms for all N from 2 up to 58. Various descriptors are used in analyzing the results, including stability, shape, and similarity functions, as well as radial distances of the atoms and the orbital energies, all as functions of N. Also, dissociation patterns and the symmetry of the clusters are analyzed. By comparing with results of jellium calculations and with those of earlier embedded-atom studies, it is demonstrated that, for gold clusters, electronic effects are very important, leading to a partial suppression of the occurrence of magic numbers, as well as to a low symmetry partly compact clusters. Also, shell-like structures are found. It is suggested that stability of gold to form strong binding in low-coordinated systems is the reason for the occurrence of planar and shell-like structures.

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Molecular hydrogen storage systems: a first-principles study

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A sustainable provision of energy is one of the greatest challenges to mankind. Energy generated from sustainable sources has to be transported and stored in an efficient and ecologically friendly way. Hydrogen is an important energy carrier in current sustainable energy scenarios. Such scenarios are only realistic, however, if hydrogen can be stored in a light, compact, fast and reliable way, and under moderate conditions. Here, hydrogen storage properties of a number of promising molecular systems and nanomaterials are investigated by first-principles calculations [1].

We first consider polylithiated carbon and oxygen molecules and study their interactions with hydrogen molecules. For polylithiated molecules it is found that the Li atoms connected to a central C or O atom, bear substantial positive charges. Hydrogen molecules are then clustered around these Li atoms via electrostatic interactions. According to our calculations such molecules can attach hydrogen up to ~40wt% with average hydrogen binding energies between 0.1 and 0.2 eV/H2. To prevent clustering of polylithiated molecules, we attach them to (doped)graphene. The now immobilized molecules have a similar interaction with hydrogen molecules as free molecules. Naturally, the hydrogen weight percentages are then reduced to 5–8wt% due to the additional weight of the graphic templates [2].

As an alternative storage system, we consider the boron sheets that have recently been proposed as novel structures [3]. Direct interaction of molecular hydrogen with the naked boron sheet is weak (0.05 eV/H2), similar
to the interaction with graphene (0.03 eV/H2). We find that dispersion of alkali metal (AM=Li, Na, and K) atoms onto the boron sheet markedly increases both hydrogen binding energies and storage capacities. The unique structure of the boron sheet presents a template for creating a stable lattice of strongly bonded metal atoms with a large nearest neighbor distance. The strong interaction between the boron sheet and the AM atoms results in a partial transfer of the AM valence electrons to the boron sheet. In particular, Li is found to be a promising doping element for the purpose of hydrogen storage. Electrostatic interactions between Li and the hydrogen molecules then lead to an average binding energy of 0.2 eV/H2, and up to a maximum of 10 wt % hydrogen [3].

In conclusion, we show that polylithiated molecules [2] or alkali metal decorated boron sheets [3] can be used as versatile building blocks for hydrogen storage materials.


Investigation of surface magnetism at atomic scale

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A very intriguing research direction is related to the physics of surfaces and interfaces. The electronic structure suffers modifications, an enhancement of magnetism and changes induced by impurities are present. By means of the spin-polarized fully relativistic screened Korringa-Kohn-Rostoker (SKKR) Green's function method, we are able to determine layer- and atom-resolved quantities. Since we calculate atomic-resolved quantities for the nanostructures, our first principles study gives the necessary insight on the fundamental physics governing the magnetic properties at the nanoscale.

For the present study I shall concentrate on the investigation of magnetic moments and anisotropies of surface-supported nanostructures of magnetic atoms, in relation to recent developments in magnetic recording media.

The exploration of ultimate density limits of magnetic information storage requires elaborate tuning of the magnetic properties, such as the easy magnetization axis, the magnitude of the magnetocrystalline anisotropy energy (MAE) and the magnetization. In order to determine the influence of the surface and interface effects on the magnetic properties of the nanostructures, we have considered several systems (Fe, Co) deposited on different non-magnetic substrates (Cu, Ir, Pt). The size of the investigated structures ranges from complete layers to single adatoms [1–3].

We demonstrate the possibility of controlling the easy magnetization axis direction and of tuning the anisotropy energy of the nanostructures.


Role of the tip in NC-AFM energy dissipation

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NC-AFM is an invaluable tool when probing surfaces, providing atomic resolution topography and detailed threedimensional force maps. As the tip scans the surface, it is common practice to record the feedback gain signal associated to the energy dissipated in the oscillation cycles. This dissipation signal often differs significantly from conventional topography images, with dissipation showing different contrast patterns, periodicity and tipsurface distance dependence. Although many different surfaces have been studied with atomic resolution in both topography and dissipation, a routine interpretation of these measurements has yet to be found. A particular problem is to devolve the influence of the tip from observed images and to really understand the atomic processes at the surface responsible for dissipate energy. In order to understand better the role of the tip is measured dissipation, we carried out extensive atomistic calculations using a wide variety of different tip materials and structures, and a simple NaCl (100) surface. Implementing our home-built virtual AFM, we simulated dissipation imaging based on the “double minimum” approximation [1]. Our calculations pointed out how ideal tips fail to give dissipation, as they are too stable to generate any atomic reconstruction, while non-ideal, defected tips allow the system to hop between two metastable configurations as the tip approaches and retracts. The statistical hysteresis in the configurations probabilities ultimately cause an hysteresis loop in the force acting on the tip, giving energy dissipation of the same order of experimental data. Alongside static dissipation simulations, we also explore fully dynamic approaches taking advantage a recent development in computational architecture.


Figure 1: System’s energy dependence on the adatom displacement for different tip heights.