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REGIONAL CENTRE OF ADVANCED TECHNOLOGIES AND MATERIALS
LECTURES

Thursday, January 22nd, 10:00 am
Seminar room of RCPTM (room No. 314), Šlechtitelů 11, Olomouc

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„Density-functional Calculations of the Magnetic Anisotropy of Nanostructured Materials"

Abstract: Nanomagnetism stands as one of the frontier field of magnetism. It offers new vista to high-density magnetic data storage devices on one hand, on the other hand many fundamental questions in nanomagnetism remain still to be answered. The design of novel devices, which functionality is engineered towards computing speed, storage capacity and energy saving, requires insight into the properties of potential materials. Theoretical methods based on density-functional theory provide an efficient tool to obtain both a thorough characterization of the materials and a better understanding of the underlying phenomena in nanomagnetism. The focus is on materials with a large magnetic anisotropy which prevents the loss of information through thermally activated magnetization reversal. A high magnetic anisotropy energy (MAE) is expected in systems with large spin and orbital magnetic moments and strong spin–orbit coupling (SOC). Hence bimetallic nanostructures in which large moments are carried by ferromagnetic 3d transition-metal atoms an heavy 5d atoms contribute to a strong SOC are promising candidates.

In this talk I will present selected results obtained during the last years of investigations of the magneto-structural properties of small transitionmetal clusters, both in the gas-phase and adsorbed on graphene, either free-standing or supported on a metallic substrate. Gas-phase transition-metal dimers are the smallest objects with a magnetic anisotropy. For homoatomic Ir2 and Pt2, and for mixed IrCo and PtCo dimers astonishingly large MAE's reaching 70 meV/dimer have been predicted. Gas-phase clusters are primarily of scientific interest, since for any practical applications magnetic nanoclusters must be deposited on a relatively inert substrate. The magnetic properties of the clusters are very sensitive to the interaction with the support. For example, for Pt2 bound to a C–C bridge site of the free-standing graphene layer spin- and orbital moments and the MAE are only reduced, but Ir2 bound in the center of a sixfold hollow is almost completely demagnetized. Isolated Pt atoms and dimers on graphene/Ni(111) are nonmagnetic, supported trimers and tetramers are weakly magnetic but the magnetic anisotropy of the cluster/support complex is dominated by that of the graphene-covered Ni(111) surface. For homoatomic Ir2 and Pt2 dimers a flat adsorption geometry on Cu(111) supported graphene5 is preferred over an upright geometry. Thus the magnetic moment of the dimer is strongly reduced and the magnetic anisotropy is very low. In contrast, for the mixed IrCo and PtCo dimers an upright configuration represents the ground state both on free-standing- and on Cu(111)-supported graphene. The mixed dimers are bound to graphene through the Co atom which magnetism (in particular the orbital moment) is strongly reduced, while due to the weaker binding within the dimer the moments are enhanced on the 5d atoms which become closer to the free-atom limit. The influence of the substrate on the magnetic anisotropy of the mixed dimers is totally different: the large magnetic anisotropy energy of IrCo is enhanced to 0.2 eV/dimer, while that of PtCo is reduced. The mechanism determining the magnetic anisotropy will be discussed in relation to the electronic structure of the dimers.