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Unusuall magnetic anisotropies in artificial surface nanostructures: nano-wires, corals and particles on Pt and Cu surfaces

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Magnetic nanostructures are often viewed as they may replace nanocrystalline materials in the quest for ever increasing density of magnetic data storage. Computational studies of these systems based on first-principles methods are nowadays possible with high accuracy on realistic system sizes. Consequently, quantities which are very difficult or currently not possible to measure can be calculated and analyzed. In this talk i present the basic building blocks of a theory and respective computational tools to calculate the magnetic properties of surface nanostructures based on a relativistic multiple scattering theory, including the description of the host surface and the embedding procedure. The theory will be illustrated by calculating various magnetic properties including Magnetic Anisotropy Energies of nanostructures ranging from single impurities to quantum corals. Since many of such systems exhibit ground states which are canted and/or non-collinear, a zero temperature spin-dynamics technique is described as an efficient method to find them. This is illustrated on Co and Fe chains on Pt(111) surface where comparison with experiment is possible. At the end i will show how general symmetry arguments can be used to extend the results of calculations.