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Magnetocrystalline anisotropy of adatoms and monolayers: an illustrative view ONDREJ SIPR, Institute of Physics of the CAS, Prague and University of West Bohemia, SERGIY MANKOVSKY, Ludwig-Maximilians-Universitat Munchen, JAN MINAR, Ludwig-Maximilians-Universitat Munchen and University of West Bohemia, Pilsen, HUBERT EBERT, Ludwig-Maximilians-Universitat Munchen — It has been known for decades that the magnetocrystalline anisotropy is linked to the spin-orbit coupling (SOC). Nevertheless, the mechanism how it arises for specific systems is still subject of debate. We focus on finding markers of SOC in the density of states (DOS) and on employing these markers for understanding the source of magnetocrystalline anisotropy of nanostructures, represented here by adatoms and monolayers. Fully relativistic ab-initio KKR-Green function calculations were performed for Fe, Co, and Ni adatoms and monolayers on Au(111) to investigate changes in the orbital-resolved DOS due to a rotation of magnetization. In this way one can see that for adatoms a significant contribution to the magnetocrystalline anisotropy comes from pushing of the SOC-split states above or below the Fermi level. A similar picture emerges from model crystal field Hamiltonian calculations. One of the consequences of this mechanism is that the magnetocrystalline anisotropy energy crucially depends on the position of the energy bands of the adatom with respect to the Fermi level of the substrate. We assume that these conclusions can be extended to nanodots and supported clusters.

Ondrej Sipr
Institute of Physics of the CAS, Prague and University of West Bohemia

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