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Structural properties of free nanoalloys and oxide-supported nanoparticles GIULIA ROSSI, Helsinki University of Technology, Espoo, Finland, ANDREA C. LEVI, University of Genoa, Italy, ZDENKA KUNTOVA, Institute of Physics, AS CR, Prague, Czech Republic, FLORIN NITA, ANDREI JELEA, CHRISTINE MOTTET, CINaM/CNRS, Marseille, France, GIOVANNI BARCARO, ALESSANDRO FORTUNELLI, IPCF/CNR, Pisa, Italy, JACEK GONIAKOWSKI, INSP/CNRS and Université Paris VI, France, RICCARDO FERRANDO, University of Genoa, Italy — The control of the structure and chemical order of metal nanoparticles is crucial in determining their properties and possible applications. We present a computational approach able to predict stable structural motifs of oxide-supported metal nanoparticles as a function of size and composition. The interaction of metal nanoparticles with the support can induce the stabilization of different epitaxies as varying cluster size. For Ag and Au the transition from cube-on-cube (001) epitaxy to (111) epitaxy is investigated. In other cases, unusual phases can be found. For example, nanoparticles with hcp structure can be stabilized for Ni, which is an fcc metal. Results are in good agreement with experimental data on Ag, Au and Ni/MgO(100) nanodots. The approach allows to derive driving forces for the stabilization of different epitaxies of metal nanoparticles on square-symmetry oxide surfaces, thus generalizing the results to a broad class of metal/oxide systems.

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