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Ab-initio determination of magnetic properties of Fe-Co nanoclusters on Cu(100). JAN ZABLOUDIL, CORINA ETZ, Center for Computational Materials Science, TU-Vienna, BENCE LAZAROVITS, BALAZS UJFALUSSY, Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, LASZLO SZUNYOGH, Center for Applied Mathematics and Computational Physics, Budapest University of Technology and Economics, PETER WEINBERGER, Center for Computational Materials Science, TU-Vienna — By making use of the fully-relativistic screened Korringa-Kohn-Rostoker method supplemented by the embedded cluster method the spin and orbital magnetic moments as well as the magnetocrystalline anisotropy energy (MAE) of Fe-Co nanoclusters of different sizes are explored as a function of the cluster composition. The MAE and magnetic moments are found to vary strongly in dependence on the concentration of Fe and Co atoms as well as on specific arrangements of atoms within the clusters. Consequently the easy magnetization axis can be tuned by controlling the cluster composition. In contrast to clusters of a pure material there exist additional contributions to the anisotropy in the surface plane due to the two different atomic species.

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