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Characteristics of Co islets on Cu(111) from first principles calculations[1] DUY LE, TALAT RAMAN, University of Central Florida — Through first principles electronic calculations, based on the spin-polarized density functional theory using the generalized gradient approximation and the ultrasoft pseudopotential method in the plane wave representation, we have examined the structure and magnetic properties of Co monomer, dimer and several n-mers on Cu(111). We find that the monomer has slight preference for the fcc site as compared to the hcp (about 0.02eV) while there is no such preference in the case of the Co dimer. The dimer bond length is found to be about 2.15?. For the 6 atoms cluster, we find that it prefers to be antiferromagnetic and absolute magnetic moment of each Co atom is about 0.07-0.08μB. The monomer is non-magnetic while a high magnetic moment of 1.94μB per Co atom is found in the case of dimer. We discuss our results in the context of recent experimental and theoretical findings [1,2]

[1] S. Borisova *et al*, Phys. Rev. B **78**, 075428 (2008)
[2] O. Mironets *et al*, Phys. Rev. Lett. **100**, 096103 (2008)

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