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H_2 dissociation of H_2 on Co layers on Cu(111) from abinitio studies[1] DUY LE, SERGEY STOLBOV, TALAT RAHMAN, 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 studied the adsorption and the dissociation of H_2 on two Co layers grown on Cu(111). As H_2 approaches the surface with the H-H bond parallel to that surface, it dissociates at a distance of about 1.7? from the Co layer, and constituent H atoms proceed to occupy neighboring fcc and hcp sites. The "adsorption" energy barrier for H_2 is 0.14 eV and the "adsorption" energy is about 0.80eV. On the Co surface, H diffuses from an fcc site to an hcp site, or vise versa, with diffusion barriers of 0.17eV and 0.12eV respectively. We find no evidence of subsurface H. By analyzing the local electronic density of state, we establish, in agreement with suggestion from experiments [1], that the surface electronic states and magnetic moment of Co atoms depend very much on the H coverage.

[1] M. Sicot *et al*, Phys. Rev. B **77**, 035417 (2008)

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