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CO adsorption on metal surfaces: a hybrid density functional study with plane wave basis set

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Abstract

We present a detailed density-functional investigation of the adsorption of CO in top and hollow sites on the (111) surfaces of Cu, Rh and Pt. The study has been performed using a conventional gradient-corrected exchange–correlation functional (the PBE functional proposed by Perdew, Burke and Ernzerhof 1996 *Phys. Rev. Lett.* **77** 3865) and two hybrid functionals mixing density-functional and exact (Hartree–Fock) exchange (the PBE0 functional of Perdew, Burke and Ernzerhof 1996 *J. Chem. Phys.* **105** 9982 and the HSE03 functional proposed by Heyd, Scuseria and Ernzerhof 2003 *J. Chem. Phys.* **118** 8207).

As expected, the gradient corrected functional shows the tendency to favor the hollow sites, at variance with experimental findings that give the top site as the most stable adsorption site.

The PBE0 and HSE03 functionals reduce this tendency. Indeed, they predict the correct adsorption site for Cu and Rh but fail for Pt. But even in this case, the hybrid functional destabilizes the hollow site by 50 meV compared to the generalized gradient approximation description. This suggests that, in general, hybrid functionals still do not predict the correct adsorption site.
