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Density functional study of CO adsorption on d-metal surface using TPSS functional JIANWEI SUN, JOHN PERDEW, Department of Physics and Quantum Theory Group, Tulane University, New Orleans, Louisiana 70118 — Feibelman *et al*[1] presented the puzzle of CO at the Pt(111) surface, showing that the LDA and Perdew-type GGA put the molecule at the wrong, high-coordination site. However, a recent study [2] showed that the BLYP yielded very satisfactory adsorption energies and the correct adsorption sites for CO adsorption on late 4d and 5d transition metal (111) surfaces, although at the price of large errors in the volume of the d metals. Since PBE and BLYP have similar accuracy, it seems the probable reason for the wrong adsorption site is due to the fact that the LDA and Perdew-type GGA's are "jellium derived" and hence prefer a more delocalized bonding, rather than that the LDA and GGA inaccurately describe the CO molecule's chemical bond. TPSS meta-GGA is also "jellium derived", but improves accuracy for molecules[3]. Therefore, as a possible candidate to identify the major reason for the wrong adsorption site, TPSS is used to calculate the adsorption energies and sites of CO on the d-metal surface in the more accurate geometric structure obtained by PBEsol[4]. [1] P.J. Feibelman *et al*, J. Phys. Chem. **105**, 4018(2001). [2] A. Stroppa and G. Kresse, New Journal of Physics **10**, 063020(2008). [3] V.N. Staroverov *et al*, J. Chem. Phys., **119**, 12129(2003). [4] J.P. Perdew *et al*, Phys. Rev. Lett., **100**, 136406(2008).

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