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Comparative study of CO adsorption on nanostructured Cu and Au surfaces FAISAL MEHMOOD, ABDELKADER KARA, TALAT S. RAHMAN, Department of Physics, Kansas State University, Manhattan KS 66502, CLAUDE R. HENRY, CRMCN, Marseille Cedex 09, France — The chemisorption of CO on Cu surfaces is regarded as a prototype system to understand molecular adsorption on transition metals surfaces. To understand the observed trends¹ in the site specific (flat, stepped, and kinked) adsorption energies of CO on Cu surfaces, we have performed a density functional theory based first principle electronic structure calculations on several low and high Miller index surfaces of Cu with CO adsorbed on-top site. Our calculated values show that adsorption energies increase with decrease in the local coordination of CO with the substrate, as seen in the experiment, although this dependence is not trivial. For in depth understanding of this, we have made a detailed study of electronic structure of these systems. Our calculated vibrational frequencies of CO-molecule on these surfaces are very similar, as expected. However, the frequency of the CO-metal stretch mode shows a small increase for the lower coordinated surfaces as compared to that on the low Miller index surfaces. Similar trends are also found for workfunctions, charge densities and the local density of states. Results will also be presented for CO adsorption on Au(111), Au(211), Au(532) and the behavior compared to that on the Cu surfaces. This work is supported in part by NSF Grant No. CHE0205064. ¹S. Vollmer, G. Witte, C. Wöll, *Cat. Lett.*, **77**, 97 (2001).

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