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Vibrational recognition of adsorption sites for CO adsorbed on transition-metal surfaces ISMAILA DABO, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, CODY FRIESEN, Department of Chemical and Materials Engineering, Arizona State University, Tempe, AZ 85287, ANDRZEJ WIECKOWSKI, Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801, NICOLA MARZARI, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139 — We have studied the vibrational properties of carbon monoxide adsorbed on transition-metal surfaces, using density-functional perturbation theory in the GGA-PBE approximation. The full dispersions for CO adsorbed on high-symmetry surface sites have been calculated, obtaining excellent agreement with spectroscopic measurements. This agreement in predicting absolute frequencies and frequency shifts as a function of the adsorption site is at variance with the poor performance of most exchange- correlation functionals in describing the energetics of adsorption. We provide a simple physical picture justifying this accuracy. These results open the possibility to directly connecting experimental vibrational spectra with the microscopic details of adsorption geometries.

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