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Energetic, structural and vibrational properties of carbon monoxide on transition-metal surfaces: a linear-response approach to the energy puzzle ISMAILA DABO, MIT, ANDRZEJ WIECKOWSKI, UIUC, NICOLA MARZARI, MIT — We have studied the energetic, structural and vibrational properties of carbon monoxide adsorbed on platinum and platinum-ruthenium surfaces using density-functional theory within the generalized-gradient approximation (GGA) and its molecular U variant (GGA + molecular U) introduced by Kresse *et al.* [*Phys. Rev. B* 68, 73401 (2003)]. Our study puts in evidence that the GGA frequency predictions for the C-O stretching mode are in excellent agreement with spectroscopic measurements. This agreement is made more remarkable by the generally-poor performance of standard exchange-correlation functionals which fail even in predicting the most stable adsorption site for CO on platinum. It is also shown that the molecular U correction to the electronic hybridizations and adsorption energies does not affect the excellent accuracy of the GGA vibrational-property predictions. Based on the linear-response approach proposed by Cococcioni and de Gironcoli [*Phys. Rev. B* 71, 35105 (2005)], we provide a theoretical justification for this observation. The accuracy of density-functional theory in predicting accurate vibrational spectra while paradoxically failing in determining correct adsorption energies is also discussed.

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