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Rethinking chemisorption: New insights into the factors controlling the binding energy[1] MARISOL ALCANTARA ORTIGOZA, SERGEY STOLBOV, University of Central Florida — Chemisorption of atomic and molecular species on a substrate induces electronic charge redistribution upon which substrate nuclei respond by adjusting their positions. This lattice distortion has been linked to the binding energy E_B of the adsorbed species and attached to the so-called surface relaxation energy, E_{rx}. We have found, however, that for transition metals the energy associated with the mere charge redistribution E_{elec} is much larger than E_{rx} and thus both contributions must be considered [1]. In this work, we quantify the electronic and structural perturbation energy E_P brought by various adsorbates on surfaces to understand anomalous adsorbate binding energies, i.e., those in which E_P strongly influences the magnitude of E_B. For example, for O adsorption on Au(111), while E_{rx} is only 0.25 eV, the overall perturbation energy E_P affecting E_B(O) is $\sim$ 1 eV [1]. This indicates that E_P cannot be ignored but also that local bonds may not be as weak as portrayed by E_B, even though E_B is significantly reduced. We expose cases in which E_P is really dominated by the lattice distortion energy, as well as a rationale for its trends as a function of the substrate and adsorbate. We discuss the implications of the fact that E_B is not always predominately controlled by the bond-strength on heterogeneous catalysis, as well as the applications of the same fact. M. Alcántara Ortigoza and S. Stolbov; "The Perturbation Energy: The missing key to understand gold 'nobleness.' " Submitted in October 2014

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