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Metal Nanoparticles Can Have Dipoles

Finding from a theoretical study provides a mechanism for substrate adsorption on catalyst surfaces

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The Pauling paradigm of chemical bonding holds that molecules made of identical atoms do not have ionic character. But a theoretical study from **Donald G. Truhlar** and Kaining Duanmu of the University of Minnesota, Twin Cities, shows that, in fact, metal nanoparticles actually can develop uneven charge distributions (*J. Phys. Chem. C* 2014, DOI:**10.1021/jp511055k**). Such particles can contain patches of partial positive charge and thereby dipole moments. This property has profound implications for catalysis—the mechanism by which a reactant adsorbs onto a heterogeneous catalyst often remains hypothetical. As a test case, Truhlar and Duanmu studied carbon monoxide oxidation employing a silver nanoparticle catalyst. The researchers calculated the electronic distributions and binding energies of silver nanoclusters containing two to 18 atoms. They found that the charge distributions can be very uneven and that the particles have large dipole moments. The areas with more positive charge provide an energetically favorable, and thus superior, adsorption site for CO. The researchers note that this property meshes well with the observation that rough edges on a catalyst substrate improve its performance: “Bumpy surfaces have more peaky atoms with more positive atomic charges, which is a previously unappreciated aspect,” they say.

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