

First principles study of CO reactivity on metallic nano particles

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The activity of a surface is determined by the local electronic structure. When nano particles are adsorbed, the catalytic properties will change. Surfaces with adsorbed nano particles often show a significantly higher chemical reactivity than the clean counterpart. Gold, for instance, shows an extra high activity towards many reactions, such as low-temperature catalytic combustion, partial oxidation of hydrocarbons and CO oxidation when dispersed as ultra-fine particles on metal oxide surfaces. In the case of CO oxidation, the activity has been observed to depend critically on the nano particle size, the nature of the support and the detailed synthetic procedure.

Since it has been observed experimentally that the chemical reactivity of a nanoparticulated surface tend to depend on the size of the adatom structures, suggesting a quantum size effect, we find it well motivated to perform a theoretical investigation with focus on the cluster-size dependence. We have chosen to model CO interaction with sodium nano particles with focus on small particles, containing only a few atoms, since we expect the eventual quantum effects to be most pronounced for these. Further, we limit our investigation to unsupported nano particles because our previous investigations [1] have shown that it is predominately states localized to the nano particle region that contribute to the local electronic structure above the particle itself. The calculations have been performed in the context of density functional theory applying the MIKA real-space program package [2], using norm-conserving pseudo-potentials for the molecule. The nano particle has been modeled as a cylindrically symmetric quantum dot. For further details, see [3,4].

Our results show that the charge transfer between the nano particle and the CO molecule depends critically on the nano particle size, and that this dependence is intimately connected to the local electronic structure at the point where the molecule approaches the particle. The key factor for charge transfer turns out to be the presence of states with the symmetry of the chemically active molecular orbital at the Fermi level.

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