ACTIVATION OF CATALYTIC PROPERTIES OF METAL NANOCLUSTERS

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S u m m a r y

Within the methods of electron density functional and *ab initio* pseudopotential, we have obtained the spatial distributions of the density of valence electrons and the electron energy spectra for metallic and oxidized small clusters from the atoms of Cu, Ni, and Co with the aim to determine the mechanisms of their high catalytic activity. We have determined a certain organization of the electronic structure of the isolated metallic (Cu, Ni, Co) atoms in the ground and excited states, which is conserved at the association of these atoms in two atomic clusters. This has allowed us to draw conclusion about the easier excitation of *d*-electrons of copper as compared with the electrons of nickel and cobalt. This provides a possible freeing of *d*-orbitals that is fundamentally important for the catalytic activity of copper centers.