Trends in CO Oxidation Rates for Metal Nanoparticles and Close-Packed, Stepped, and Kinked Surfaces

Using density functional theory calculations, we study trends in the CO oxidation activity for different metals and surfaces. Specifically, we show how the activity of (111) close-packed surfaces, (211) stepped surfaces, (532) kinked surfaces, 55 atom cuboctahedral clusters, and 12 atom cluster models changes with the coordination number of atoms at the active sites. This effect is shown to be electronic in nature, as low coordinated metal atoms, which bind reactants most strongly, have the highest energy metal d states.