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The role of ligands effect in the atomic and electronic structure of Pt_{55} and Au_{55} nanoclusters[1] DIEGO GUEDES SOBRINO, São Carlos Institute of Chemistry, Univ de São Paulo, MAURÍCIO J. PIOTROWSKI, Universidade Federal de Pelotas, JUAREZ L.F. DA SILVA, São Carlos Institute of Chemistry, Univ de São Paulo — One of the greatest problems in the use of transition-metal nanoclusters in nanocatalysis is the environment effects induced by ligands, which affects the atomic and electronic properties, and hence, their reactivity, however, our atomistic understanding is far from satisfactory due to complex nature of the ligand-metal interactions. In this talk, we will report a first-principles investigation of ligand effects (PH_3, SH_2) on the physical and chemical properties of Pt_{55} and Au_{55} using density functional theory (FHI-aims). We found that a reduced core structure ($7-10$, instead of 13), called LOW, is about 5.45 eV (2.00 eV) lower in energy than the icosahedron (ICO) model for Pt_{55} (Au_{55}) ($\Delta E_{\rm tot} = E_{\rm tot}^{\rm LOW} - E_{\rm tot}^{\rm ICO}$), which is consistent with previous results. Furthermore, spin-orbit coupling does not affect the relative stability. We found that the addition of ligands, from 1 to 18, decreases $\Delta E_{\rm tot}$ to about -0.25 (Pt_{55}) and 0.07 eV (Au_{55}) for 18 PH_3 ligands, and -0.10 (Pt_{55}) and 0.17 eV (Au_{55}) for SH_2 ligands. We observed an average increase of about 0.70% in the bond lengths due to the ligand effects, however, it affects only slightly the coordination number.

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