COMPUTATIONAL STUDIES OF NEW SUPRAMOLECULAR GOLD INTERACTIONS

Daniel Blasco

e-mail: daniel.blasco@helsinki.fi; daniel.blascos@unirioja.es

The concept of *metallophilicity* encompasses attractive van der Waals interactions between pairs, strings, or clusters of closed- (d^{10}, s^2 d^{10}) or seemingly closed-shell (d^8) late transition metals that originate from the relativistic mass increase of the s electrons. Among metallophilic interactions, *aurophilicity* has a privileged status due to its noticeable strength of 30-50 $kJ \cdot mol^{-1}$ that affects the crystalline structure and bulk properties of gold(I)-containing materials. The character of the interaction is supported by ever-growing irrefutable structural evidence and by computational simulation at post-Hartree-Fock (HF) and density functional theory (DFT) levels. In this seminar, the chemical nature of our recently proposed gold(I)-lanthanide(III) bond will be discussed from a theoretical viewpoint. Furthermore, a new computational proof for the existence of the elusive gold(III) aurophilicity will be presented.