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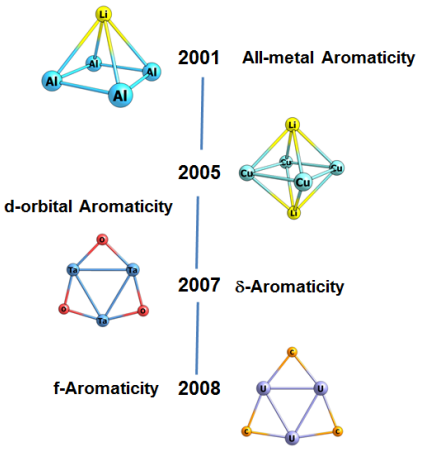
Chemical bonding and aromaticity in novel inorganic and organometallic clusters

CANIOC

Clusters behave as a link between the atom and the bulk material. Their properties strongly depend on their size. Such nanoparticles can be potentially useful for many technical applications. The structural characterization of clusters is essential to understand the changes in their size-dependent properties. Experiments alone provide an incomplete picture of the cluster structure. In fact, a combination of theory and experiment is essential to get a complete description of these nanoparticles. Understanding the chemical bonding and aromaticity of these clusters is essential to fine tune their properties in the quest of new materials with enhanced non-linear optical properties, increased oxidant character, or improved charge transfer separation needed to construct more efficient solar cells.



In the CANIOC project we have analyzed the chemical and aromaticity of supermolecular flowers, five-membered metallacycle rings, nanoclusters made of iron, cobalt and nickel in different proportions, and $[M_2N_2]^{2-}$ (M = B, Al, Ga), $[M_2N_2]^{2+}$ (M = C, Si, Ge, Sn, Pb), E_2P_4 (E = B, Al, Ga, In), and $CN_3Be_3^+$ and $CO_3Li_3^+$ clusters. The CANIOC project has represented a great advance towards the design of novel clusters with fascinating properties.