Towards a molecular-level understanding of fluxional metal atomic clusters. Recent case studies.

Content

The very recent development of highly selective techniques making possible the synthesis and experimental characterization of atomic metal clusters is pushing our understanding far beyond the present knowledge in materials science, driving these clusters as a new generation of quantum materials at the lower bounds of nanotechnology. When the size of the metal cluster is reduced to a small number of atoms, the d-band of the metal splits into a subnanometric d-type molecular orbitals network in which all metal atoms are inter-connected, with the inter-connections having the length of a chemical bond (1−2 Å). These molecular characteristics are at the very core of the high stability and novel properties of the smallest metal clusters, with their integration into colloidal materials interacting with the environment having the potential to further boost their performance in applications such as luminescence, sensing, bioimaging, theranostics, energy conversion, catalysis, and photocatalysis. Through the presentation of very recent case studies, my talk is aimed to illustrate how first-principles modelling, including methods beyond the state-of-the-art and an interplay with cutting-edge experiments, is helping to understand the special properties of these clusters at the most fundamental molecular-level. First, I will be shown how the application of first-principles methods have disclosed the fundamental reasons why Cu5 clusters experience a reversible oxidation [1], including aggregation and support effects [2], and are capable of increasing and extending into the visible region the solar absorption of TiO2, of augmenting its efficiency for photo-catalysis beyond a factor of four, also considering the decomposition and photo-activation of CO2 as a prototypical (photo-)catalytic reaction. Finally, I will discuss how the modification of the same material with subnanometric Ag5 clusters has converted it into a "reporter" of a surface polaron property as well as a novel two-dimensional polaronic material.

[1] M. P. de Lara-Castells, J. Colloid Interface Sci. 312, 737-759, (2022).
[2] J. Garrido-Aldea and M. P. de Lara-Castells, *Aggregation and support effects in the oxidation of fluxional atomic metal clusters. The paradigmatic Cu5 case* (2022) submitted.

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