Ab initio modelling of materials: role of surfaces in reactivity

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Ab initio techniques allow exploring the structure-properties relationships without empiric parameters, and its combination with experimental characterization becomes a powerful tool in the design of materials with selected applications. I will present three examples of application:

- the spectroscopic properties of TiO_2: despite the wide use of titanium dioxide materials, some aspects of their optical properties are poorly known. I will present the research conducted in the group to elucidate structure-response relationships as regards photoactivity and unexpected behavior observed on titania-based materials.
- the study of materials at the nanoscale: the properties of nanosized materials, mainly the control of shape in metallic nanoparticles and the structural evolution cluster – nano – bulk in TiO_2 will be discussed. Insights obtained from the chemical bond analysis tools will be presented.
- the development of catalysts with enhanced redox properties: the purification of hydrogen for its use in fuel cells needs specific redox catalysts, among the most selective are the ceria-based materials. Doping ceria with gallium enhances considerably the reducibility of the material and the ability to split H_2, opening new perspectives for hydrogenation reaction over metal oxides in the absence of noble metals.

References

Photoactivity of molecule-TiO_2 clusters with Time-Dependent Density-Functional Theory
E. Luppi, I. Urdaneta, M. Calatayud
J. Phys. Chem. A 120 (2016) 5115–5124 DOI: 10.1021/acs.jpca.6b00477

Understanding How in situ Generated Hydrogen Controls the Morphology of Platinum Nanoparticles
N. Aguilera-Porta, M. Calatayud, C. Salzemann, C. Petit J. Phys. Chem. C, 118 (2014), 9290–9298

Promoted ceria catalysts for alkyne semi-hydrogenation
G. Vile, P. Dähler, J. Vecchietti, M. A. Baltanás, S. Collins, M. Calatayud, A. Bonivardi, J. Perez-Ramirez

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