Magnetism in Pt-nanoparticles

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Nanoclusters are today of widespread use in various applications, ranging from nanomedicine to memory storage, nano-optics, plasmonics, and catalysis. Such a broad spectrum of applications is possible because of the delicate interplay between electronic structure and geometrical features in the absence of any translation symmetry, allows their peculiar and novel chemo-physical properties to be tunable by cluster architecture (size, shape, chemical composition and ordering) and by nanoparticles' interaction with the surrounding environment. Unraveling the difficult shape-property relationship is indeed at the core of the so-called "bottom-up" approach. In the attempt of clarifying and exploiting the dependence of chemo-physical properties on cluster architecture, atomistic modeling based on density-functional theory offers a very powerful and detailed tool as we can manipulate and control nano-objects at the atomic scale *in silico*. In this talk, we are going to show how the magnetism arising in nano-sized Pt objects is due to a geometrical effect present in the second coordination shell and it is enhanced in twinned shapes. We also demonstrate how magnetism is affected by the environment in the case of small Pt-nanoclusters embedded in zeolite pores. Among the 50 stable isomers in the gas phase, due to geometrical constraints, only about 1/3 of those clusters can be inserted in the zeolite pores. Severe structural rearrangements occur depending on whether the solid angle at the Pt vertex bound to the super-cage, for example, the icosahedron reconstructs into a lower coordinated morphology. The high magnetic moment of Pt13 in a zeolite, is mainly due to four highly coordinated shapes -truncated bi-pyramid; a triaugmented triangular prism; two incomplete double icosahedra- which represent the 30% of the sample in the hypothesis that all the isomers have the same probability to be inserted in the pore.

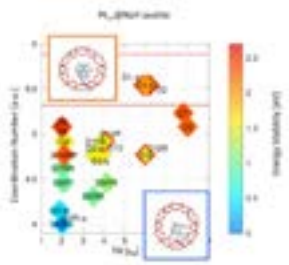

Figure 1 Total magnetisation and coordination of Pt13 inserted into a zeolite pore. Colours refer to energy stability.

Biography

Roberto D'Agosta has completed his PhD in 2003 from Roma Tre University. Then he moved to the University of Missouri, Columbia in the group of Professor G Vignale from 2003-2005 and then at the Physics Department, University of California, San Diego in the group of Professor M Di Ventra as Research Assistant since 2008. Then he moved to San Sebastian as Visiting Professor in Autumn 2008 and there he was offered a Ikerbasque Research Professorship starting in April 2009 at the University of the Basque Country (EHU/UPV), a position he holds now. Although his research is mainly in the field of Thermoelectric Materials, he then collaborated with Thomas Young Centre (London) and then with Dr. F Baletto's group at KCL, he brought his expertise in density functional theory to the study of magnetic materials.

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