Università degli Studi di Trieste

Dipartimento di Fisica

Seminario

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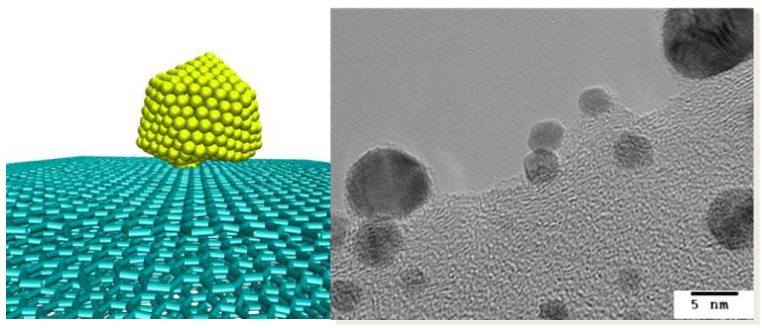
Wednesday, November 16, 5:00 PM - Lecture Room A, F building, Dip. di Fisica – via Valerio 2 – Trieste

HRTEM & X-ray Absorption Spectroscopy meets atomistic modeling to understand structure and properties of metal clusters and nanoalloys



In materials science, the range of properties of metallic systems can be greatly extended by taking mixtures of elements to generate intermetallic compounds and alloys. In many cases, there is an enhancement in specific properties upon alloying due to synergistic effects, and the rich diversity of compositions, structures, and properties of metallic alloys has led to widespread applications in electronics, engineering, and catalysis. Nanoalloys are also of interest as they may display structures and properties which are distinct from those of the pure elemental clusters: the structures of binary clusters may be quite different from the structures of the corresponding pure clusters of the same size; synergism is sometimes observed in catalysis by bimetallic nanoalloys. They may also display properties which are distinct from the corresponding bulk alloys due to finite size effects.

The understanding of the interaction of metals clusters and nanoalloys with its environment (ligands molecules, substrate surface, etc) is crucial to develop new catalytic materials at the nanoscale.

In this talk, we will demonstrate how HAADF-STEM images, electron microscopy simulations, X-ray Absorption Spectroscopy and computer simulations (Molecular Dynamics, grand canonical Monte Carlo and DFT calculations) can be used as complementary techniques to understand the structure, thermodynamics and growth mechanism of metal clusters & nanoalloys.

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Everyone interested in the topic is welcome to attend

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