AVVISOS DI SEMINARIO

Giovedì 11 luglio 2013 alle ore 12.00 nell’aula A1 del DSCF (ed C11)

il professor IAN P. HAMILTON

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terrà un seminario su

**Gold Clusters and Nanostructures: Zero Kelvin and Finite Temperature Calculations**

*Tutti gli interessati sono invitati a partecipare.*

*Il Direttore del Dipartimento*

*Prof. Silvano Geremia*

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**Abstract**

Gold clusters and nanostructures (Au$_n$, $n = 1$-40) are studied theoretically (at zero Kelvin) using standard density functional theory methods. The Kohn-Sham equations are solved for the valence electrons and scalar relativistic effects are incorporated via a pseudopotential. For larger $n$ values, at zero Kelvin, many structural isomers are stable including compact, helical nanorod and cage geometries. We consider adsorption of, and reaction with, various small molecules. The effect of finite temperature can be extrapolated using the vibrational modes of the structural isomer.

For various structural isomers, finite temperature stability is examined theoretically using a constant temperature density functional theory molecular dynamics approach as implemented in the FHI-aims (Fritz Haber Institute *ab initio* molecular simulations) code. [1,2] Here the Kohn-Sham equations are solved for all the electrons and scalar relativistic effects are incorporated via the ‘atomic-ZORA (Zeroth Order Regular...
Approximation). The electrons are treated quantum mechanically but the nuclei are treated classically. At room temperature, cage geometries are typically more stable than alternate structural isomers such as the compact and helical nanorod geometries that were the subject of a recent theoretical study. [3]

Au_{24} Cage Structure, 300K, 26ps

References:

