UNIVERSITÀ
DEGLI STUDI DI TRIESTE

DIPARTIMENTO DI FISICA

Friday December 11, 2015 - 2:00 p.m.

Miramare Campus – Leonardo Building, Room 204

Modeling Thiol-Gold interface for protected nanoparticles

Numerical model implementation on a convenient computational platform

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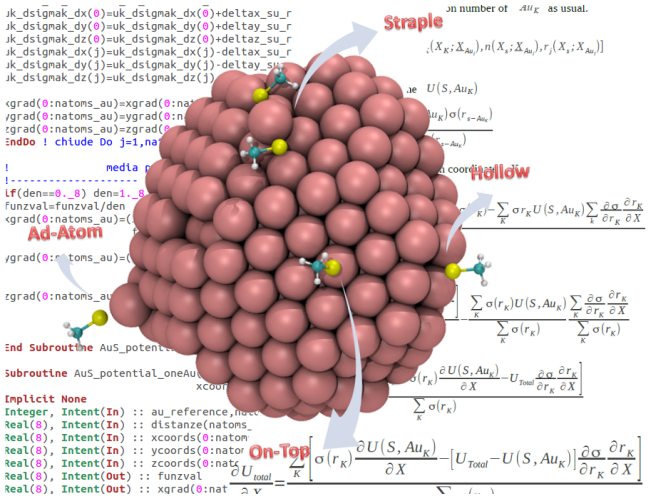
Self-assembled monolayers (SAMs) are applied to gold nanoparticles to guide growth, increase stability, and provide additional functionality. However, as with any surface coating, the changes to the energetics of the surface can have unanticipated consequences, as well as can introduce new opportunities. Understanding the relationship between the coverage degree and type of the SAMs and the underlying gold nanoparticles is challenging, but can be explored very efficiently using modeling and computational simulations. In that sense, very recently we have developed a semi-empirical many-body potential, fitted from DFT calculations, which takes account many different absorption sites for MethilThiolate on Gold Surfaces.



Ministero degli Affari Esteri e della Cooperazione Internazionale

Organized by M. Peressi within the Project "Supported metal nanoparticles for catalysis, hydrogen storage and other technological applications: numerical modelization for an optimal design" co-funded by MAECI