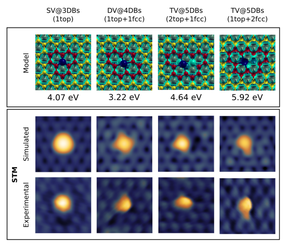
THEORETICAL AND COMPUTATIONAL CONDENSED MATTER PHYSICS

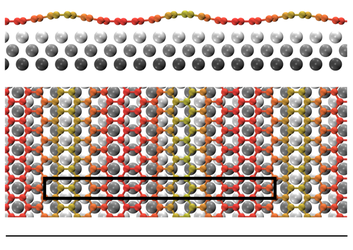
dipartimento di TRIESTE fisica

SURFACES & THIK FILMS

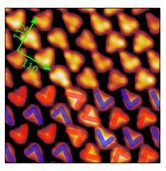
Graphene defects



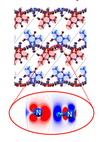
Graphene/Ni(001)

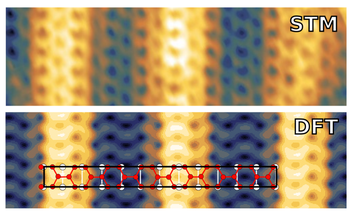


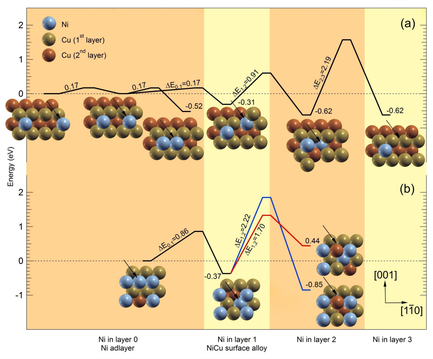
Theophylline on Au(111)



Charge rearrangment within the layer

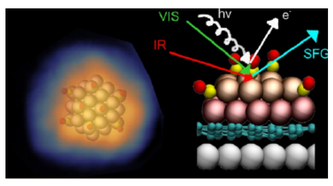




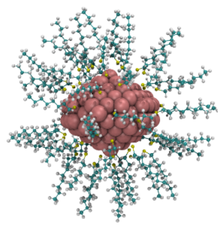


NANOPARTICLES & NANOWIRES

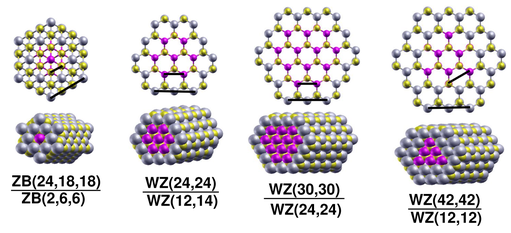
Pt cluster/Graphene/Ir(111)



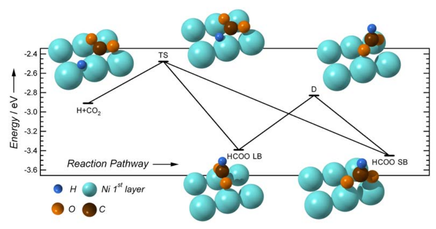
Thiols on Gold Nanoparticle



Nanowires



NANOCATALYSIS



ELECTRONIC STRUCTURE OF MATERIALS

Prof. Maria Peressi (peressi@ts.infn.it)

What?

The group is involved in experiments making massive use of atomic-scale numerical simulations of real materials using quantum mechanical first principle Density Functional Theory and semi-empirical (Molecular Dynamics, Kinetic Monte Carlo) approaches.

Why?

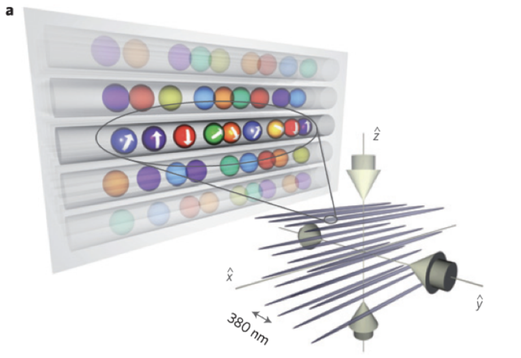
- To predict structural, electronic, magnetic and reactivity properties of materials and physical/chemical processes.
- To interpret experimental results.

Ongoing collaborations:

- CNR-IOM TASC Laboratory (prof. G. Comelli, dott. C. Africh, dott. E. Vesselli)
- Universidad Nacional de Cordoba, Argentina (prof. M. Mariscal)

THEORY AND SIMULATION OF CONFINED FERMIONS

Prof. Gaetano Senatore (senatore@units.it)



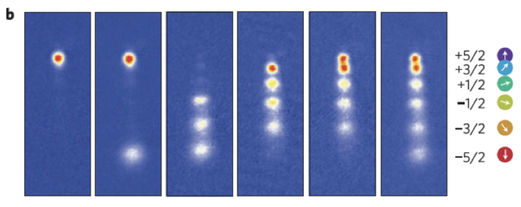
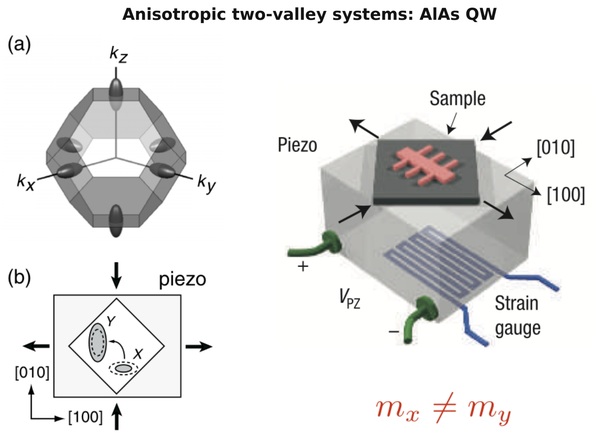


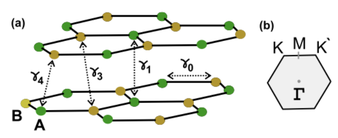
Figure 1 | Ultracold 1D fermionic liquids with tunable spin. a, A 2D optical lattice is used to create an array of independent quantum wires of ultracold ^{173}Yb with six possible nuclear spin orientations. **b**, The nuclear spin of the atoms can be manipulated with optical pumping techniques, resulting in a tunable number of spin components, and analysed with optical Stern–Gerlach detection (see Supplementary Information).

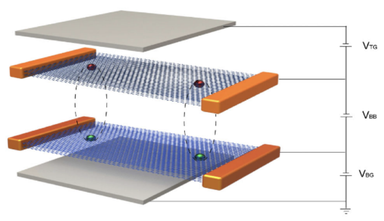
A)



B)

C)





Current research projects:

A) Multi component (spin) systems $1 \leqslant 2S+1 \leqslant 6$

B) Effects of $m_x/m_y \neq 1$ and $2S+1$ on magnetism

C) Dependence of excitonic condensation on $2S+1$

Tools:

- Quantum Monte Carlo simulation
- Many-body techniques

Collaborations:

IOM-CNR Democritos (S. De Palo and S. Moroni)

LIQUID AND COLLOIDS

Prof. Giorgio Pastore (pastore@ts.infn.it), prof. Enrico Smargiassi (enrico.smargiassi@ts.infn.it)

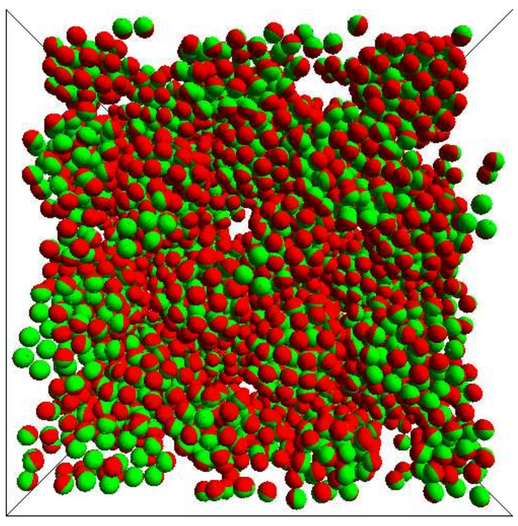


Fig. 1. Instantaneous configuration of a colloidal system of Janus type: red faces are purely repulsive interactions, while green-green alignement results in a square-well attraction.

What?

Theoretical and computational research into various fields of liquid state physics, with a special interest for colloids.

Topics & Collaborations:

- Studies of the correlations, and dynamic and thermodynamic properties of models for colloidal systems. This line of research has emerged from the extension of classical approaches to the theory of liquids (such as RHNC-type integral equations) to include the short-range anisotropic interactions (Kern and Frenkel model), and good agreement has been obtained with simulation data.
  Collaborations with A. Giacometti (Padua), F. Lado (NC State University) and F. Sciortino (Rome).
- Ab-initio (DFT) studies and modeling interactions with polarizable effetive potentials in molten salts and ionic liquids. Recent studies have looked at applications on halides of group 12 metals.
- Liquid-glass transition studied within the Random First Order Transition theories. Collaboration with Jean-Marc Beaumont, Univ. Metz, e Jean Pierre Hansen, Univ. Jussieu, Paris.

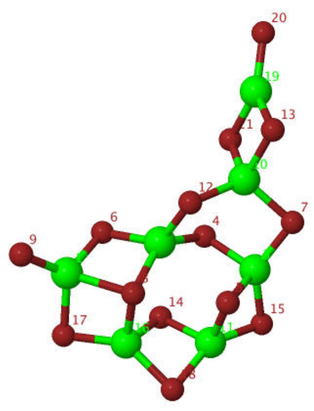


Fig. 2. Local minumum configuration of a heptamer cluster of $ZgCl_2$. Preference for the bulk tetrahedral coordination motif is already visible in such a small cluster. The local minimum predicted by a polarizable potential has been confirmed by ab-initio calculations.