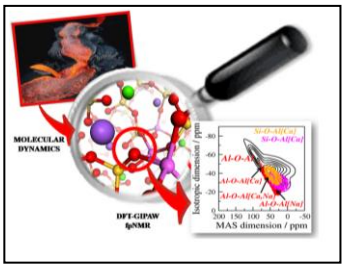
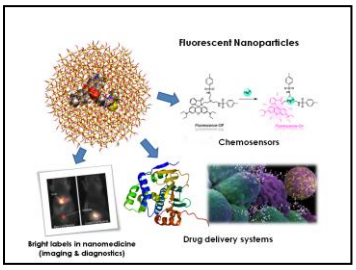
Computational Chemistry Group

Material & Life Science

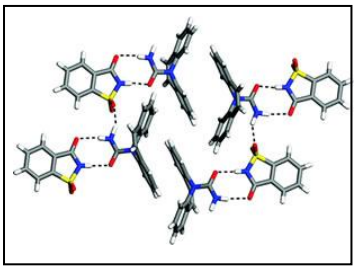
Alfonso Pedone, Gianluca Malavasi & Maria Cristina Menziani



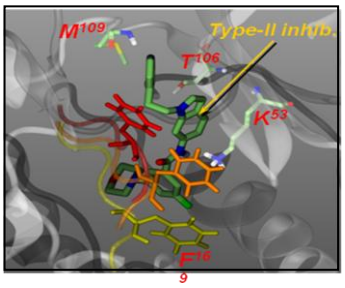
Oxide Glasses



Nanoparticles



Molecular Crystals



Proteins & Drug Design

CONTACTS

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Sito web del gruppo

PEOPLE

The research group is composed by Prof. M. C. Menziani (associate professor), Dr. Alfonso Pedone, (researcher), Dr. G. Malavasi, Dr. Francesca De Rienzo (Technician) and three PhD Students (Dr. Marta del Cadia, Dr. Elisa Gambuzzi, Dr. Davide Presti).

SKILLS

The group scientific and technological expertise is in the field of theoretical and computational chemistry of small molecules, inorganic nanomaterials, and complex biological systems. The domains of competence of our group include: 1) ab initio methods, in particular density functional theory (DFT) 2) molecular mechanics and classical molecular dynamics 3) hybrid QM/QM and QM/MM methods, and 4) Car-Parrinello Molecular dynamics.

RESEARCH TOPICS

Oxide Glasses. Disordered inorganic materials are being increasingly used for addressing major technological challenges in energy, medicine, and advanced communication systems. Computational simulations provide a unique atomic scale picture of the structure of glasses allowing us to address the crucial question for the development of such materials, i.e. an improved understanding of their fundamental structure-property relationships.

Nanoparticles. Fluorescent nanoparticles hold considerable promise for technological applications in biochemical, bio-analytical, and medical areas. Theoretical studies can provide valuable information on the structural, dynamical, photophysical and spectroscopic properties of dye-doped silica nanoparticles and metal nanoparticles functionalized with biological molecules.

Molecular Crystals. Organic molecular crystals play very important roles in many industries, including pharmaceuticals, agrochemicals, pigments, dyes, explosives and electronics. We are particularly interested in the theoretical description of the polymorphism of these materials since it affects their overall key properties such as shelf-life, solubility, morphology and stability.

This research activity is part of a collaborative project among the universities UNIPR, UNIMORE, UNIBO, and UNIFE founded by Emilia-Romagna “SPINNER 2013 PER I DOTTORATI DI RICERCA”

Proteins & Drug Design. Computational simulations and prediction of structure, function, protein-protein, protein-ligand, protein-environment interactions and development of Quantitative Structure-Property Relationships (QSPR) are performed with the aim of rationalizing and interpreting experimentally observed behavior at the molecular level, design new molecules, and suggest further lines of experimental inquiry.

COLLABORATIONS

Dr. T. Charpentier (Commissariat à l'Energie Atomique, IRAMIS), Dr. A. Tilocca (University College of London. UK), Prof. P. Ugliengo, Dr. B. Civalleri (University of Turin), Prof. A. N. Cormack (Alfred University, NY, USA), Maria J Ramos (University of Porto)