Il Gruppo Nazionale di Mineralogia, con il patrocinio della Società Italiana di Mineralogia e Petrologia, organizza due giornate di studio sul tema:

Modelling the mineralogical world: how and why

14/15 giugno 2016

Dipartimento di Scienze della Terra, Aula "Sergio Lucchesi"
Sapienza Università di Roma
Piazzale Aldo Moro 5, 00185 Roma

KEYNOTE TALK: **A. R. Oganov** (SUNY –Stony Brook)

Relatori: **C. Angeli** (UNIFE), **D. Belmonte** (UNIGE), **M. Bruno** (UNITO), **M. Faccenda** (UNIPD), **M. Merli** (UNIPA), **C. Stangarone** (UNIPR)

Comitato scientifico*:*

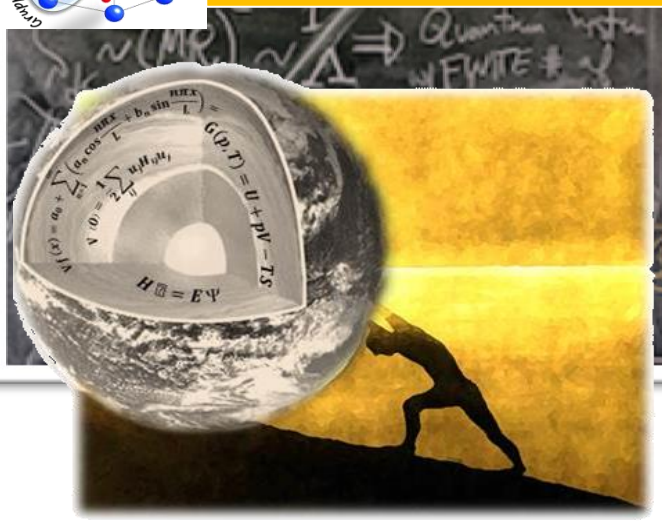
Paola Comodi (UNIPG)
Annalisa Martucci (UNIFE)
Marco Pasero (UNIPI)
Mauro Prencipe (UNITO)
Gabriella Salviulo (UNIPD)

Comitato organizzatore:

Giovanni B. Andreozzi (UNIROMA1)
Paola Comodi (UNIPG)
Annalisa Martucci (UNIFE)
Marco Pasero (UNIPI)
Mauro Prencipe (UNITO)
Gabriella Salviulo (UNIPD)

La partecipazione alla giornata è gratuita.
Per questioni organizzative, si prega di inviare una manifestazione di interesse via e-mail (all'indirizzo marco.pasero@unipi.it) entro il 20 maggio.
Un secondo avviso, contenente maggiori dettagli, sarà distribuito a fine maggio.

Modelling the mineralogical word: how and why



Celestino Angeli – Modelling the diffusion process in microporous materials: environmental and technological impacts

Microporous materials have a large interest in many environmental and technological applications, where the key aspect is the diffusion process within the material. The theoretical description of this process is a complex task because the standard Fick equation is inadequate and a more involved formulation, namely the Maxwell-Stefan equations, must be used. A numerical strategy for the solution of these equations will be shortly sketched out and a few applications are described concerning the permeation across a microporous membrane and the uptake and displacement kinetics on a microporous material.

Marco Bruno - On the simulation of the crystal surfaces

The understanding of surface and interface properties is essential to deepen our knowledge in a variety of pure and applied research. Nowadays, there are not analytical methods able to determine unambiguously the structure of a crystal face, as well as it is not possible to perform experimental measures to obtain the thermodynamic properties of a surface. A fundamental contribution to such a study is given by the quantum-mechanical, semi-empirical and empirical simulations, which allow to individuate the most stable structure of a surface and calculate their thermodynamic properties.

Marcello Merli – Catastrophes in the electron density: what happens to a crystal when it approaches the phase transition point

The deep mechanism of the transformation of a crystalline form to another is examined via a Bader's topological analysis of the electron density coupled with the Thom's catastrophe theory. We will see why a structure is no longer stable near the transition point, i.e., what catastrophic event happens to the electron density. Some examples of catastrophes in minerals will be shown.

Artem R. Oganov - Discovering new materials, minerals and phenomena with evolutionary algorithms

Thanks to powerful evolutionary algorithms, in particular the USPEX method, it is now possible to predict both the stable compounds and their crystal structures at arbitrary conditions, given just the set of chemical elements. Recent developments include major increases of efficiency and extensions to low-dimensional systems and molecular crystals and new techniques called evolutionary metadynamics and Mendelevian search. Some of the results that I will discuss include:

1. Theoretical and experimental evidence for a new partially ionic phase of boron, γ-B and an insulating and optically transparent form of sodium.
2. Predicted stability of "impossible" chemical compounds that become stable under pressure – e.g. Na_3Cl, Na_2Cl, Na_3Cl_2, $NaCl_3$, $NaCl_7$, Mg_3O_2 and MgO_2.
3. New chemistry of planet-forming systems Mg-Si-O and N-H-O.
4. Novel surface phases (e.g. boron surface reconstructions).
5. Prediction of new ultrahard materials and computational proof that diamond is the hardest possible material.

Donato Belmonte – *Ab initio* thermodynamics of deep mantle processes: the mineral physics perspective

In this talk I will focus on how first principles theory and computational thermodynamics could reveal mineral behaviour and phase equilibria in the deep mantle of the Earth. Some common assumptions made on planetary-scale processes will be also discussed and revisited from the perspective of mineral physics.

Manuele Faccenda – Petrological numerical modelling of the convective Earth

Numerical simulations of the Earth's internal dynamics rely on the experimentally and numerically determined physical properties and phase relationships of the most abundant minerals found in nature. In this contribution we will explore the state-of-the-art numerical techniques used in geodynamics for realistically reproducing the physical and mineralogical behavior of Earth-like planets.

Claudia Stangarone – Unravelling vibrational frequencies of crystal lattices: quantum mechanical approach and possible application in Planetary Science

In this talk, I will show a new approach in the study of vibrational frequencies of crystal lattices, which is particularly useful in the interpretation of Raman and IR spectra of minerals, as the established accuracy of computational *ab initio* methods in the validation, interpolation and prediction of experimental data, has been definitely proven. Moreover, I will show how this approach can be used in planetary sciences