



Italian Society of Mineralogy and Petrology

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MODELLING THE MINERALOGICAL WORLD: HOW AND WHY

GNM Workshop – Roma, 14–15 June 2016

A workshop on the use of computational methods in mineralogical sciences – Modelling the Mineralogical World: How and Why – which was organized by the National Mineralogical Group (GNM), an informal group within the aegis of the Italian Society of Mineralogy and Petrology (SIMP) was held 14–15 June 2016. Both SIMP and the Italian Society of Geochemistry (SoGel) sponsored the workshop, and SIMP also provided financial support.

The workshop took place in the Department of Earth Sciences at the Sapienza University of Roma (Italy), in a room named after the recently deceased Sergio Lucchesi, who was professor of mineralogy at Sapienza.

Artem R. Oganov (Stony Brook University, New York, USA) was the keynote speaker and he presented a fascinating lecture addressing how to predict “impossible compounds” just on the basis of chemical composition and how such compounds might become stable under an increase in pressure, the new chemistry of the planet-forming chemical systems Mg–Si–O and N–H–O, and on the modelling of new ultra-hard materials.



(A) Prof. A. R. Oganov giving his opening lesson.
(B) Prof. Oganov relaxing with some of the workshop's participants.



Other talks were given by a variety of speakers from Italian universities. Celestino Angeli (University of Ferrara) spoke on diffusion processes operating through microporous materials and how to model them by applying Maxwell–Stefan equations. Donato Belmonte (University of Genova) spoke on the use of first principle theory and computational thermodynamics in the study of deep mantle processes. Marco Bruno (University of Torino) spoke on how to model crystal surfaces using quantum-mechanical, semi-empirical or empirical simulations. Manuele Faccenda (University of Padova) spoke on how to numerically model the petrology of a convective mantle in Earth. Marcello Merli (University of Palermo) spoke on how to determine electron densities during phase transitions via the use of catastrophe theory. And Claudia Stangarone (University of Parma) spoke on the use of vibra-



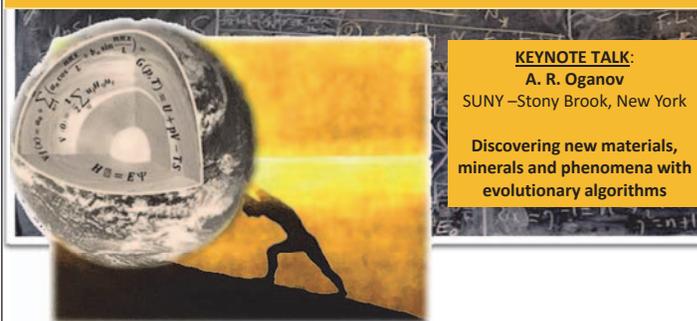
The organizing committee with the Director of the Earth Science Department at Sapienza University. FROM LEFT TO RIGHT: A. Martucci (Ferrara University), M. Prencipe (Torino University), M. Pasero (Pisa University), P. Comodi (Perugia University), G. Scarascia Mugnozza (Sapienza University, Roma).

tional frequencies of crystal lattices in the interpretation of Raman and infra-red (IR) mineral spectra. During their spare time, participants had the chance to visit the historic mineralogical collections in the museum at Sapienza University.

This workshop was targeted at PhD students and young researchers and, with more than 50 people attending, can be said to have been a great success. Participants and organizers also had the great pleasure of welcoming to the event, as a special guest, the now 94-year-old retired professor of mineralogy, Marcella Federico.

Modelling the mineralogical world: how and why

June 14–15, 2016, Department of Earth Sciences,
Sapienza University of Roma
“Sergio Lucchesi” room



KEYNOTE TALK:
A. R. Oganov
SUNY –Stony Brook, New York

Discovering new materials,
minerals and phenomena with
evolutionary algorithms

Speakers:

- Celestino Angeli** (University of Ferrara, Italy) – Modelling the diffusion process in microporous materials: environmental and technological impacts,
- D. Belmonte** (University of Genova) – *Ab initio* thermodynamics of deep mantle processes: the mineral physics perspective
- M. Bruno** (University of Torino) - On the simulation of the crystal surfaces
- M. Faccenda** (University of Padova) – Petrological numerical modelling of the convective Earth
- M. Merli** (University of Palermo)– Catastrophes in the electron density: what happens to a crystal when it approaches the phase transition point
- C. Stangarone** (University of Parma) – Unravelling vibrational frequencies of crystal lattices: quantum mechanical approach and possible application in Planetary Science



Scientific Committee

P. Comodi University of Perugia, Italy ; A. Martucci University of Ferrara, Italy ; M. Pasero University of Pisa, Italy ; M. Prencipe University of Torino, Italy; G. Salviulo, University of Padova, Italy

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