



New ideas on the behaviour of minerals in Earth's mantle and core

A.R. Oganov, F. Zhang

(1) Laboratory of Crystallography, Department of Materials, ETH Zurich, Wolfgang-Pauli-Str. 10, CH-8093 Zurich, Switzerland.

(2) Geology Department, Moscow State University, 119992 Moscow, Russia.

Knowledge of material properties at conditions of the Earth's deep interior is necessary for meaningful interpretations of seismological data and for realistic geodynamical modelling. In the recent years, computational mineral physics has made major advances, some of which will be discussed in this talk:

1. Finite-temperature calculations of the elastic constants, and their applications for the interpretation of seismic tomography maps [1].
2. Calculations of mineral phase diagrams from first principles, and their implications for Earth's composition, structure and dynamics [2,3]. One particular example here is the post-perovskite phase of MgSiO_3 , the predicted stability field of which has guided its experimental synthesis, and has important geophysical consequences [3].
3. Novel approaches for studies of mineral plasticity, which have clarified the origin of seismic anisotropy in the deep mantle [4].
4. Novel evolutionary methodology for the prediction of stable crystal structures at given pressure-temperature conditions, which has resulted in the prediction of several new mineral phases at conditions of the deep interiors of the Earth and terrestrial planets [5,6]. We will discuss potential core-forming alloys and

novel mineralogy of carbonates (and the possibility of their decomposition) in the mantle.

References

1. Oganov A.R., Brodholt J.P., Price G.D. (2001). The elastic constants of MgSiO_3 perovskite at pressures and temperatures of the Earth's mantle. *Nature* **411**, 934-937.
2. Oganov A.R., Gillan M.J., Price G.D. (2005). Structural stability of silica at high pressures and temperatures. *Phys. Rev.* **B71**, art. 064104.
3. Oganov A.R., Ono S. (2004). Theoretical and experimental evidence for a post-perovskite phase of MgSiO_3 in Earth's D" layer. *Nature* **430**, 445-448.
4. Oganov A.R., Martoňák R., Laio A., Raiteri P., Parrinello M. (2005). Anisotropy of Earth's D" layer and stacking faults in the MgSiO_3 post-perovskite phase. *Nature* **438**, 1142-1144.
5. Oganov A.R., Glass C.W., Ono S. (2006). High-pressure phases of CaCO_3 : crystal structure prediction and experiment. *Earth Planet. Sci. Lett.* **241**, 95-103.
6. Oganov A.R., Glass C.W. (2006). Crystal structure prediction using evolutionary algorithms: principles and applications. *J. Chem. Phys.* **124**, art. 244704.