Ab initio treatment of minerals at high pressures and temperatures

D.Y. Jung [1,2], A.R. Oganov [2], [1]Institute of Mineralogy and Petrology, Department of Earth science, [2]Laboratory of Crystallography, Department of Materials, ETH Zürich, Switzerland, daniel.jung@erdw.ethz.ch

The mantle of the Earth extends from the depth of about 670 km to 2981 km. It consists mainly of $MgSiO_3$-perovskite, (Mg,Fe)O magnesiowüstite and $CaSiO_3$-perovskite. It is possible to calculate thermodynamic properties, structures and energetics of the separate minerals at extreme conditions of the mantle using *ab initio* methods. To get a better picture of the mantle it is necessary to not only look at chemically pure minerals, but to consider them as solid solution, as it is the probable case in nature.

The calculations are based on the generalized gradient approximation (GGA) [1] method and the projector augmented wave (PAW) method [2], which is a very accurate method for solving the total energy problem.

Using density functional theory the structure and the stability of the $CaSiO_3$ perovskite in the pressure range of the Earth's mantle (0-150 GPa) have been calculated [3]. Additionally we use the subregular solid solution model together with point defect calculations to model the solidus curve of the (Ca,Mg)-perovskite phase diagram at 25 GPa. This is a special case, because there is also a symmetry change from a tetragonal to an orthorhombic perovskite structure as you increase the concentration of Mg. This is the first work to treat this subject with ab initio methods.

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References:

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