***Ab initio* treatment of minerals at extreme conditions**

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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, such as the density functional theory with the generalized gradient approximation (GGA) [1] and the projector augmented wave (PAW) method [2], which are included in the VASP [3] code. To get a better picture of the mantle it is necessary to not only look at chemically pure minerals, but to consider them as a solid solution, as it is the probable case in nature.

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 [4]. Additionally we use the subregular solid solution model together with point defect calculations to model the solvus 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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