

Ab initio modeling of thermal chemical properties of the core-mantle boundary region

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The physical properties of minerals are definitely key to understanding the deep Earth interior. Even though accurate experimental measurements are still difficult, *ab initio* density functional theory can alternatively provide some substantial information at ultra-high pressure and temperature conditions. In particular, *ab initio* thermodynamics and elasticity are very useful for the quantitative modeling of seismological properties and to analyze the thermal chemical properties of the deep Earth. For example, discontinuous jumps and subsequent reductions observed in typical one-dimensional seismic S velocity models of the core-mantle boundary region can be reconciled by the post-perovskite phase change in MgSiO_3 with subsequent velocity reductions along superadiabatic temperature increase. Our recent investigations suggest a reverse phase change is less requisite for this, which constrains the CMB temperature to be relatively low leading to relatively small CMB heat flux. Also typical tomographic lateral velocity variations in the S-wave may be interpreted mostly by the phase change within only a few hundred lateral temperature variations. On the other hand, in some places, strong chemical heterogeneity also needs to be assigned, which might be related to the possible existence of some heavy primordial materials.