Insights into the Properties of the Deep Earth from Computational Mineral Physics

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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 [2-4]. 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 [4].
3. Novel approaches for studies of mineral plasticity, which have clarified the origin of seismic anisotropy in the deep mantle [5].
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 [6,7].

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