Theory and Computation for High-Pressure Mineral Physics

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Abstract

Recent progress in theoretical mineral physics (TMP) based on the density functional quantum mechanical theory has been dramatic in conjunction with the advancement of computer technologies. It is now possible to predict high-P,T equation of state and phase stability of complex minerals quantitatively with uncertainties that are comparable to or even smaller than those attached in experimental data. The technique is now routinely applied not only for theoretical backup to experiments but also for guide to experiments [1]. Our next grand challenges include new technical developments for high-P,T thermophysical and thermochemical properties, such as thermoelasticity [2], thermal conductivity [3], elemental diffusivity [4], chemical partitioning of both solid and liquid phases [5] within the correlated systems. Thermoelasticity and thermal conductivity, which are calculated based on the harmonic and anharmonic lattice dynamics theories, are keys to clarifying compositional and thermal properties of the deep mantle and core through interpreting seismological information, respectively. Chemical partitioning, which we can access using the thermodynamic integration method, on the other hand allows us to link mineral physics to geochemistry. In this talk I will report recent activities in the Ehime Univ. TMP group. References:

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