THE GEODYNAMICS SEMINAR Nº 547

Dr. Taku Tsuchiya

Professor

Geodynamics Research Center

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Venue: Zoom

A link will be sent @grc-all within 30 minutes before the beginning of the seminar.

Core-mantle chemical interactions

Chemical reaction and associated element partitioning between liquid iron and silicate melt are major processes controlling Earth's chemical evolution. Those could be expected to occur during the core formation, at the boundary between the basal magma ocean and the outer core, and also at the present core-mantle boundary through the partially molten ultra-low velocity zones, and closely related to several important solid Earth problems from the primordial reservoirs, the core and mantle chemistries, the volatile circulations, etc. Numerous experimental efforts have been made so far in geochemistry to understand the properties of reactions under high-pressure and high-temperature conditions corresponding to Earth's deep interior. However, considerable inconsistencies are often seen in different experiments likely due to the technical difficulties in precise handlings and analyses of tiny samples. Theoretical assessments are therefore substantial, in particular, the ab initio technique, which can predict energetics of materials highly quantitatively even at high P,T, might be a powerful one. Within the theoretical framework, chemical reactions are dealt with based on thermodynamics, namely free energy. Since free energy of liquid states is not easy to calculate, we adopted the special thermodynamic integration method founded by statistical mechanics. The new technique developed has been applied to metal/silicate partitioning of heat producing elements, noble gases, other volatiles, and indicator elements of the core-mantle interaction, and opened a fresh research direction combining theoretical mineral physics and geochemistry. I would introduce some results in this talk.