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Science Research Bldg. 1, 4th floor.
Ehime Univ.

Keywords:

1. Mantle Properties
2. DFT
3. Defects

The Importance of Point Defects on processes in the mantle

All minerals in the Earth contain some amount of point defects. While some of these are high in concentration (such as ferrous iron in various minerals) most are very low in concentration- of the order of ppm or less. These defects are difficult to detect and monitor and are generally ignored when considering the properties of these minerals. Despite this, some point defects can, even when small in number, have tremendous effects on properties of mantle minerals. Such properties can often behave “strangely” and thus need to be explicitly considered to derive properties of the mantle.

In this talk I shall discuss the use of ab-initio calculations and thermodynamic modelling to examine the effects of defects on the properties of the mantle. As a specific example I will discuss the effect of hydrogen based point defects on various properties and phase transformations across the mantle. This class of defect has non-Arrhenius, often nonmonotonic responses to temperature and pressure and I will show how they need to be explicitly considered when discussing the mantle.