Understanding the atomistic nature of defects in minerals: A case study of water and boron in olivine

Joshua MUIR

State Key Laboratory of Ore Deposit Geochemistry, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang , China

Defective elements hosted in minerals are extremely important throughout the earth and the universe. These defect elements can control the properties of minerals, can track the history of the mineral and can be important in forming new phases such as important ores. Understanding these defects, however, is very difficult due to their often small concentrations (in case of point defects) or complex structures (in case of grain boundaries and dislocations) which makes both experimental and theoretical examination difficult. In this talk I shall discuss how defects in minerals can be examined through a combination of *ab-initio* calculations and thermodynamics using a case study of water and boron in olivine. I shall demonstrate how understanding the atomistic distribution and nature of point defects in olivine is critical for understanding its large scale properties such as its strain rate and its conductivity.