

5th International Special Lecture

第5回グローバルCOE(第11回GRC)国際レクチャー

-Dr. Bijaya Karki's Lecture Series No.2-

July 25 (Wed), 2012 14:00-17:00

Meeting Room #486, 4F Science Research Bldg 1

Lecturer: Dr. Bijaya Karki

Interim Division Chair and Associate Professor Computer Science and Engineering in School of Electrical Engineering and Computer Science, Louisiana State University

First principles computer simulation and visualization studies of silicate liquids

The study of magma-forming silicate liquids has long been a major topic in computational geochemistry/geophysics. A wide range of properties of silicate liquids including structure and speciation, thermodynamics of mixing, isotope fractionation, chemical diffusivity, viscosity, etc. can now be studied within the framework of density functional theory. In recent years, we have simulated a series of liquids including MgO-SiO₂ binary using the first principles molecular dynamics method, and this talk will focus on the calculated melt structural and transport properties and their visualization-based analysis. Our study suggests that the melt properties are strongly dependent on pressure and temperature. The local coordination (such as Si-O coordination) and degree of polymerization dramatically increase on compression. Self-diffusion and viscosity coefficients vary by several order of magnitudes over relevant pressure-temperature ranges, even showing dynamical anomalies in some cases. Compositional effects including those of water are found to be substantial as well. Interactive visualization of atomic position-time series allow us to associate the predicted complex dynamical behavior with the structural changes occurring on compression and to understand the microscopic origin of compositional effects. Finally, I will discuss important implications for magma dynamics.

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