Thermochemical solution properties of silicate liquids at extreme conditions and implications for the magma ocean.

Alfred Wilson*[1]

[1]UCL Earth Sciences (UCL ES) – WC1E 6BT UK, United Kingdom

Abstract

All planetary bodies are evolved from a history of accretionary impacts, delivering mass and energy to an otherwise geologically closed system. These impacts generate melting proportional to impactor size. In the case of our moon formation, despite uncertainties regarding the nature of impact and subsequent satellite formation, widespread melting would have been unavoidable. Gaining a better understanding of the properties of a molten mantle system may allow us to contemporarily identify remnants of the magma ocean, in addition to learning how the present-day system evolved. However, the process by which the magma ocean crystallized is still uncertain, including the temperature of liquidus and solidus, crystallization sequence, and compositions of crystallizing phases. Here we take a novel approach towards constraining multi-component freezing equilibria via first principles moleculcar dynamics simulations. Our initial focus has been on computation of the entropy of silicate liquids. The entropy is inaccessible to standard molecular dynamics methods and is therefore a crucial missing ingredient in the first principles computation of phase equilibria. We have investigated methods of computing the two-body configurational entropy deficit, initially focusing on the MgSiO3-CaSiO3 join. We show results for the absolute entropy and the entropy of mixing across the mantle pressure-temperature regime.

*Speaker