

Evolution of the Early Earth



Dr. DENG Jie
(鄧傑博士)

University of California, Los Angeles

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The Earth's first a few hundreds of millions of years witnessed its rapid evolution from a hot magma ocean world to a habitable planet conducive to life. The origin of life on Earth seems to demand a highly reduced early atmosphere to form bio-essential organic molecules. The redox state of the early Earth, however, remains enigmatic.

In this seminar, I will present the results of *ab initio* molecular dynamics simulations and thermodynamic modeling on the redox controlling reactions during the early phase of planetary formation when the planet was mostly molten to form the magma ocean. Based on these results, I propose a model to show that Earth's early atmosphere before core formation was oxidized, unfavorable to prebiotic synthesis of organic compounds.

This model, however, is limited to the period before the completion of the core formation. In my current research, I seek to explore the effects of subsequent magma ocean solidification on mantle redox. As a first step, I focus on resolving the poorly constrained fundamental parameters in modeling the thermochemical evolution of the magma ocean. I will show that, by leveraging the state-of-art machine learning technique and density functional theory, some important thermochemical parameters are, for the first time, rigorously determined, paving the way to understanding mantle solidification, redox evolution, and the early atmosphere of rocky planetary bodies.



Enquires: 3943 9624 essc@cuhk.edu.hk