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Jianguo Du, Baohua Zhang, Bo Zou, Bin Chen, Geeth Manthilake

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## Editorial

## High pressure geochemistry: Preface



The origin and history of the Earth are manifested as the evolutionary processes of chemistry and physics of its interiors, which can be recognized by deciphering the geochemical signals recorded in minerals and rocks. Deep interiors of the Earth and other rocky planets are under both extreme pressure and temperature, i.e., approximately 360 gigapascals (GPa) and as high as 7000 K at the center of the Earth. So far, many questions on Earth's interiors remain equivocal, such as the compositions and mineralogy of the mantle and core, the causes of chemical and physical heterogeneities of the mantle, origins of magma and petroleum, the role of fluid-rock interaction in the crustal evolution and earthquake generation, the behavior and partition of elements and chemical species, chemical dynamics of the degassing process, among other processes, which have attracted much attention of scientists. The materials in the interior domains of Earth and other planets experience the extreme processes of high pressure and high temperature (high  $P$ - $T$ ) conditions. Not only does high temperature, but also high pressure severely affects the behavior of atoms and molecules, chemical dynamics of reactions, and existing states of materials. However, traditional investigations usually neglect the chemical reactions under high  $P$ - $T$  conditions. Thus, the high  $P$ - $T$  chemical reactions and processes are among the most important factors in the Earth's evolution, which are involved in various geological processes, such as mantle metasomatism, element differentiation, isotopic fractionation, magma evolution, ore formation, alteration of rocks, earthquake generation, etc. Therefore, studies of the geochemical behavior of materials under high  $P$ - $T$  conditions are fundamental to understand the physicochemical properties of the Earth's interior. High-pressure experiments and theoretical simulations are powerful tools to explore the Earth's interiors in addition to the geophysical techniques, analysis of natural samples and meteorite. This Special Issue of High Pressure Geochemistry in *Geoscience Frontiers* assembles contributions that present results of high pressure geochemistry, concerning mainly the behavior and partition of elements, hydration and dehydration of minerals, origin of magma, reaction between minerals and magma, effect of chemical composition (as well as volatiles) on the transport property of mineral/rock, gas diffusion, phase transitions and occurrence states of materials under high  $P$ - $T$  conditions.

Chemical interaction between melts and mineral, partial melting of rocks show new evidence for the origin of magmas. The experimental work on dehydration and partial melting of amphibolite at 1.5 GPa

and 800–950 °C revealed that the melt was geochemically similar to adakite, indicating the origin of adakite that is widely distributed in the eastern North China Craton (Ye et al., 2020). The trace element data of the experiment reaction products under high  $P$ - $T$  conditions indicated that the high-SiO<sub>2</sub> OIB type of basalts with variable chemical compositions could be originated from reaction between basaltic melt and orthopyroxenite (Zang et al., 2020).

Chemical compositions, hydration and dehydration of minerals greatly contributed to heterogeneity of the mantle. The experimental study of natural epidote up to 17.7 GPa and 700 K implied that the cold subducting slab might carry epidote into the upper mantle and the dehydration of epidote may be one potential cause for the 410 km seismic discontinuity (Li et al., 2020). Phase relation experiments in the MgSiO<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> system indicated that bridgmanite, the most abundant phase in the lower mantle, could contain 30 mol% Al<sub>2</sub>O<sub>3</sub> at 27 GPa and 3000 K, and the solubility of Al<sub>2</sub>O<sub>3</sub> in bridgmanite increased with increasing temperature, informing our understanding of the dynamics of the shallow part of the lower mantle (Liu et al., 2020a). The investigation of synthesized  $\delta$ -(Al<sub>0.95</sub>Fe<sub>0.05</sub>)OOH crystals up to 135 GPa indicated that the incorporation of 5 mol% iron increased the volume of  $\delta$ -AlOOH by 1%–2%, but decreased the shear-wave velocity ( $V_S$ ) by ~5% at 20–135 GPa, which presumably contributed to the D" layer at the bottom of the lower mantle (Su et al., 2020).

The experiments of thermal and electrical properties of minerals and rocks provided new insights into the mantle. The measured thermal properties of serpentinized harzburgite and dunite from Tibet up to 823 K and pressures up to 3 GPa indicated that thermal diffusivity ( $D$ ) and thermal conductivity ( $k$ ) systematically decreased with increasing temperature, but increased with increasing pressure. Subsequently, numerical simulation indicated that serpentinization may severely reduce  $D$  and  $k$  of rocks in subduction zone and eventually hindered temperature homogenization between subducting slabs and surrounding mantle (Ge et al., 2020). Studies of the silica-coated materials under high-pressure are essential to explore the physical and chemical properties of the upper mantle. The structural variations and optoelectronic properties of core-shell halide perovskites (CsPbBr<sub>3</sub>@SiO<sub>2</sub> NCs) may provide a new 'lithoprobe' to detect the upper mantle (Fu et al., 2020). The measurements of realgar by in situ Raman spectroscopy and the electrical conductivity indicated that realgar underwent isostructural phase transition at 6.3 GPa and then metallized phase transition occurred at 23.5 GPa, which contributed to the sulfur and arsenic recycling in the Earth (Yang et al., 2020a).

The studies of existing states of H, He, N and O in some crystals under high  $P$ – $T$  conditions provided new insight in the chemical and physical properties of the deep mantle and stars. The investigations for solid solution of pyrite-type  $\text{FeO}_2$  and  $\text{FeO}_2\text{H}$  highlighted the chemical states for O and H atoms, storage of volatile and light elements, and chemical heterogeneity in the deep lower mantle (Hu and Liu, 2020). At high-pressure, the malachite structure was stabilized by highly distorted  $[\text{CuO}_6]$  induced by hydrogen bond, and the mechanism for the phase transition in  $[\text{OH}]$ -carbonates up to 18.2 GPa was revealed, offering clues for transporting crustal carbon into the deep Earth (Gao et al., 2020). The simulations of iron nitrides up to  $\sim 70$  GPa at ambient temperature indicated that  $\text{Fe}_4\text{N}$  was stable at the experimental pressures and the incorporation of N effectively reduced the density, incompressibility, electrical and thermal conductivities of iron, which favored the understanding of the relative phenomena in the deep Earth (Zhuang et al., 2020). The prediction of HF-He system using the *ab initio* evolutionary algorithm USPEX package revealed that  $\text{HHe}^+$  could not exist at pressure  $< 1000$  GPa due to a conflict between the covalent component in symmetric hydrogen bond and ionic  $\text{HHe}^+$ . Chemical pressure from He induced the formation of  $\text{He}_2(\text{HF})_4$  with an aromaticity-like electronic behavior and unexpected ultra-large band gaps  $> 13$  eV at 900 GPa (Wang et al., 2020).

The behavior of gases in minerals under high  $P$ – $T$  conditions provided a window into the initial migration of gases in the minerals and the process of mantle degassing. The simulations for high  $P$ – $T$  adsorption behaviors of supercritical  $\text{CO}_2$  in magnesite pores indicated that the excess adsorption amounts of  $\text{CO}_2$  in the pores of magnesite decreased with increasing temperature, but increased with increasing pressure and pore size (Yang et al., 2020b). The incorporation and diffusion behavior of He in quartz and coesite were investigated by the DFT and CI-NEB methods at pressures up to 12 GPa, revealing that the diffusivity of He was anisotropic in the crystals, and the diffusivity of He in the coesite decreased with pressure. He initially escaped from those minerals significantly contributes to the mantle degassing (Liu et al., 2020).

The high  $P$ – $T$  experiments of chemical change of organic matter offered new clues for hydrocarbons existing in the mantle. The n-hexane and cyclohexane under high  $P$ – $T$  conditions tended to dehydrogenate by cyclization and graphitization, resulting in the formation of some unsaturated compounds and finally the graphitic products (Yang et al., 2020).

The C–O and O–H structures in  $\text{K}_2\text{CO}_3$  aqueous solutions of different molarities were quantitatively characterized by the features of Raman and Infrared (IR) spectroscopies, which can be applied to study  $\text{CO}_3^{2-}$ -bearing fluid inclusions (Ma et al., 2020).

We hope that the selected set of papers presented in this special issue of *Geoscience Frontiers* provide a cross-section of the state-of-the-art in high pressure geochemistry, and that these works would entice further studies on this topic.

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Jianguo Du is a professor at the Institute of Earthquake Forecasting, China Earthquake Administration and the adjunct professor at University of Chinese Academy of Sciences, China University of Geosciences (Beijing) and University of Science and Technology of China. He has been engaged in geochemical research of oil and natural gas, underground water, soil gases, and studies of fluid-rock interaction, rock/mineral mechanics, earthquake generation since 1985. He was awarded the Special Government Allowance of the State Council in 2000.



Baohua Zhang received his Ph.D. in geophysics from University of Science and Technology of China (USTC) in 2009. Then he joined Institute for Planetary Materials, Okayama University as postdoctoral for three years. Since from 2020, he is a full professor in the School of Earth Sciences, Zhejiang University. His main research interests focus on experimental studies of the transport properties (such as electrical conductivity, diffusion, thermal conductivity, etc.) of mantle minerals and rocks under high-temperature and high-pressure conditions.



Bo Zou is a professor of State Key Laboratory of Superhard Materials, Jilin University, China. His research interests concern high-pressure chemistry. Using high pressure technology, some controversial issues in science at ambient pressure have been solved. He proposed the concept of pressure-induced emission (PIE). His work is supported by National Science Foundation for Distinguished Young Scholars.

Jianguo Du  
*United Laboratory of High-Pressure Physics and Earthquake Science, Key Laboratory of Earthquake Prediction, Institute of Earthquake Forecasting, CEA, Beijing 100036, China*  
\*Corresponding author.  
E-mail address: [jianguodu@hotmail.com](mailto:jianguodu@hotmail.com)

Baohua Zhang  
*Key Laboratory of Geoscience Big Data and Deep Resource of Zhejiang Province, School of Earth Sciences, Zhejiang University, Hangzhou 310027, China*

Bo Zou  
*State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China*

Bin Chen  
*Hawaii Institute of Geophysics and Planetology, School of Ocean and Earth Science and Technology, University of Hawaii at Manoa, Honolulu, HI 96822, USA*

Geeth Manthilake  
*Laboratoire Magmas et Volcans CNRS, IRD, OPGC, Université Clermont Auvergne, 63000 Clermont-Ferrand, France*



Bin Chen is an Associate Researcher in the Hawaii Institute of Geophysics and Planetology, School of Ocean and Earth Science and Technology, University of Hawaii at Manoa, Honolulu, Hawaii, USA. He works on the physics, chemistry, and thermo-chemical evolution of the deep interiors of the Earth and Earth-like planetary bodies, through direct probing of microscopic properties of planetary materials under pressure-temperature conditions pertinent to planetary interiors. He employs both multi-anvil presses and diamond-anvil cells for generating high pressures and temperatures and often combines them with various laser, X-ray, and micro-analytical techniques for his research. He was the recipient of J. C. Jamieson Award in 2010 from the Gordon Research Conference (Research at High Pressure) and the

Faculty Early Career Development (CAREER) Award (2016–2021) from the USA National Science Foundation.



Geeth Manthilake is a senior scientist affiliated with the French National Center for Scientific Research (CNRS). Currently he is the principal scientist at the French National High-Pressure Research Platform at the Laboratoire Magmas et Volcans, Clermont-Ferrand, France. He has obtained his Ph. D. from Institute for Planetary Materials, Okayama University in 2008. Before joining the CNRS in 2012, he has completed his post-doctoral studies at the Bayerisches Geoinstitut, Germany. His research interests include transport and elastic properties of the material under high pressure and temperature conditions.