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Topic Insights

Deep Volatiles as the Key for Energy and Environments of the Four-Dimensional Earth System

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Carbon, hydrogen, oxygen, nitrogen, sulfur, and their compounds are volatile components that dominate the thin and fragile atmosphere, hydrosphere, and biosphere on Earth's habitable surface. However, the vast majority of these volatiles are hidden in the deep interior, where the high pressure–temperature conditions drastically and categorically alter the physics and chemistry of the volatiles. Like the bloodstream of an organism, the circulations and interactions of volatiles in the deep Earth modulate climate, resources, energy, natural hazards, and other factors that define the Earth as a unique living and changing planet. During the past 4.6 billion years, deep volatiles have been modifying and regulating the chemistry and temperatures of the atmosphere and oceans, thus mediating the emergence, evolution, and extinction of life. Likewise, their behaviors and changes in the future will affect the fate of our species. A better understanding of deep-volatiles will improve our ability to forecast their impacts, plan economic development, and protect the environment.

The Deep Volatiles, Energy, and Environments Summit (DVEES 2018) explored the topic of Earth's deep volatiles from the perspectives of four Science Communities—Extreme Physics and Chemistry, Reservoirs and Fluxes, Deep Energy, and Deep Life—and included sessions on allied topics such as computational studies, carbon and hydrogen under extreme pressures, and the lower mantle mineral physics. This special issue of *Engineering* contains contributions in all of these areas.

Schiffries et al. discuss a decade of discoveries by Deep Carbon Observatory (DCO) scientists on the physical, chemical, and biological roles of carbon in Earth. The vast majority of previous research on the global carbon cycle focuses on the small fraction of Earth's carbon that is at or near the planet's surface. In contrast, the DCO's overarching mission is to understand Earth's *entire* carbon cycle, including the vast majority of Earth's carbon residing in the planet's deep interior. The DCO provides a new model for tackling large-scale, interdisciplinary, and international science questions.

Field and analytical studies of natural samples have revealed fundamental constraints on deep volatiles. In this special issue, Liu and Li demonstrate that stable isotopes of calcium (Ca), magnesium (Mg), and zinc (Zn) have extraordinary potential for elucidating the fate of marine carbonates during subduction, which has profound implications for the deep carbon cycle. Anomalies of Ca, Mg, and Zn isotopes in basalts have been attributed to recycling of crustal carbonates into the mantle sources region; however, Liu and Li evaluate other processes that can potentially fractionate isotopes in the same direction as expected by carbonate recycling. Guo et al. describe large, ultra-deep oil and natural gas resources, and discuss the hydrocarbon sources and accumulation methods. New seismic acquisition and processing technologies have led to breakthroughs in the high-precision and high-resolution seismic imaging of ultra-deep reservoirs, which have enabled the discovery of ultra-deep hydrocarbon resources. Feng et al. describe metabolic features of Bathyarchaeota, which is one of the most abundant microorganisms on Earth and is ubiquitously distributed in diverse habitats, including the deep subsurface biosphere. The ancestral analysis by Feng et al. indicates a hot origin for this archaeal phylum.

Natural diamond is formed under high pressure–temperature conditions and is a unique messenger from the depth. The unparalleled strength of diamond acted as a rigid capsule that entrapped fluid and solid inclusions and preserved the valuable condition of their formation. Lian and Yang describe microdiamonds and other high-pressure phases in ophiolites, providing a new window for probing carbon cycling in the deep mantle. Ophiolite-hosted diamonds are characterized by light carbon isotopic compositions, which are interpreted as evidence of the recycling of surface-derived organic matter into the mantle. Sobolev et al. report that higher hydrocarbons (pentane to hexadecane) and their derivatives are dominant species in certain fluid inclusions in diamond, garnet, and olivine from diamondiferous peridotites from the Udachnaya pipe in Yakutia, Russia, and suggest that such hydrocarbons are major species in some mantle fluids.

Natural samples become increasingly rare with depth, and totally unavailable beyond the depth of 700 km. Experimental studies and advances in instrumentation development at central facilities are essential for rapid progress in our understanding of deep matter and energy. Zhang et al. describe the unique capabilities of *in situ* high-pressure multigrain X-ray diffraction using synchrotron radiation for exploring multiphase systems under the pressure–temperature conditions of Earth's deep interior. This powerful technique enables robust phase identification and structure determination of the individual grains in a multiphase

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assemblage contained in a diamond anvil cell. Zhang et al. have applied this technique to a wide range of important problems, such as detecting the breakdown of iron (Fe)-bearing bridgmanite, identifying the hexagonal hydrous (HH) phase in (Fe,Al)OOH, and determining the crystal structures of (Mg,Fe)SiO_3 post-perovskite (pPv) and seifertite (SiO_2) under Mbar (1 bar = 0.1 MPa) pressures. Mao et al. demonstrate that coupling nanoscale X-ray transmission microscopy (nanoTXM) with a diamond anvil cell creates exciting opportunities for non-destructive three-dimensional imaging of materials at high spatial resolution under extreme conditions. For example, Mao et al. show that *in situ* high-pressure nanoTXM can be used to determine equations of state for materials that are difficult to characterize by X-ray diffraction or micron-scale X-ray tomography at a synchrotron facility. Ishii et al. report a breakthrough in pressure generation by a Kawai-type multi-anvil press with tungsten carbide anvils, which can provide a sample that is three orders of magnitude larger than those of diamond anvil cells. These scholars have increased the pressure generated by this apparatus to 65 GPa, which is more than 2.5 times higher than the previous record for this device. Navrotsky shows that many outstanding problems in Earth and materials science will benefit from advances in and integration of three approaches: experimental thermodynamics, structural investigations, and computational methods. The integration of these approaches is beginning to provide a new understanding of stability and reactivity in complex solids, with important applications for minerals under extreme conditions and the structure of planetary interiors. Kong and Lee present experimental results on the carbonation of chrysotile under subduction zone conditions, which improve our understanding of the role of serpentine minerals in the deep carbon cycle. Binns et al. describe structural studies on the copper–hydrogen (Cu–H) system under compression, which has applications for hydrogen storage.

Computational research and data science complement other approaches for investigating deep matter and energy. Tse describes first-principles methods for investigating the chemical and transport properties of materials under extreme conditions. He provides a wide range of geological applications, including: the stability of iron-rich halides in the Earth's core, which provides a potential solution to the missing halogen paradox; the chemical behavior of CO_2 and SiO_2 under mantle conditions; water formation in Earth's upper mantle; the viscosity of $CaCO_3$ melts; and the thermal conductivity of periclase. Hazen et al. establish that large and growing data resources are ushering in a new era of data-driven discovery in mineralogy. New data-driven approaches—including mineral evolution, mineral ecology, and network analysis of mineralogical systems—address the distribution and diversity of minerals through space and time. These strategies are fostering a deeper understanding of mineral co-occurrences and facilitating predictions of undiscovered mineral species that occur on Earth.

Recent high pressure–temperature experiments and theories have revealed that the Earth's deep lower mantle (deeper than 1800 km) to the center of the core (5280 km depth) is governed by fundamentally different chemistry and physics from the outer shells: The iron can split water, making the core-mantle boundary a colossal hydrogen generator and oxygen reservoir [1]. This perpetual source of hydrogen, along with hydrogen's reactions with other volatiles to form ammonia, water, and hydrocarbons, provide essential ingredients for life as well as organic energy resources. The oxygen reservoirs are detectable as the seismic anomaly of the D″ layer at the core-mantle boundary [2]. Accumulations of the oxygen reservoirs to a critical saturation point would eventually lead to oxygen outbursts that provide an internal mechanism for sporadic or periodic global catastrophes and offer a unified hypothesis for major events throughout geological history [1]. Geodynamically, the oxygen outbursts added a chemical superplume convection driving force to the thermal convection, and could be responsible for the rifting and merging of supercontinents. Petrologically, the additions of volatile components in the superplume would lower the melting temperature of upper-mantle rocks and generate large igneous provinces (LIP). Environmentally, the rise of excess oxygen would lead to the great oxidation event and the snowball Earth, which would cause biological mass extinctions. The multidisciplinary approach to the deep volatiles issue is thus the key for understanding the four-dimensional Earth system.

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