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Editorial: Earth Deep Interior: High-Pressure Experiments and Theoretical Calculations From the Atomic to the Global Scale

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Editorial on the Research Topic

Earth Deep Interior: High-pressure Experiments and Theoretical Calculations from the Atomic to the Global Scale

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This Research Topic, hosted by Frontiers in Earth Science, responds to the eighth "From Atom to Earth" Symposium on High-Pressure Science and Earth Science, held at the Institute of Geochemistry, Chinese Academy of Sciences (IGCAS), Guiyang, China between July 2 and 5, 2021. Professor Lidong Dai from the IGCAS Key Laboratory of High-temperature and High-pressure Study of the Earth's Interior (HTHPSEI) was the conference president. Since 2007, this symposium has been organized as a major platform for Chinese scientists in the high-P research field to share their latest progress and discoveries in the field of physicochemical properties of minerals and rocks at high-temperature and high-pressure conditions. This time, 156 Chinese scholars and researchers from Peking University, Nanjing University, the Chinese Academy of Sciences, etc., participated in the conference. Of these delegates, 65 gave oral presentations, and professors Xi Liu, Duanwei He, Lidong Dai, Chun-An Tang, and Zizheng Gong delivered conference speeches (**Figure 1**). As distinguished and invited delegates, professors Hongsen Xie and Heping Li attend this conference. CAS Key Laboratory of HTHPSEI, together with IGCAS and the Chinese Society of Mineralogy, Petrology, and Geochemistry, provided the conference service.

The Research Topic contains ten papers including nine original studies and one review article reporting on the physicochemical properties of minerals and rocks obtained by using high-temperature and high-pressure experiments and theoretical calculations. The experimental studies mainly focus on high-P crystallographic features, electrical conductivity properties, and the partial melting of minerals and rocks. The theoretical calculations mostly investigate crystalline structures and rock physical parameters including crack density, fluid saturation, scalar field, charge density, and layer charge distribution, etc.

In their review, Berrada and Secco focus on research progress for electrical resistivity of Fe and Fe-alloys from the laboratory-based high-P experiments using diamond anvil cell, multi-anvil press, and shock compression equipment, as well as from first-principles calculations. Special attention is paid to the effects of some light elements (Si, S, O) on the electrical resistivity

FIGURE 1 | Group photo for the eighth “From Atom to Earth” Symposium on High-Pressure Science and Earth Science held in IGCAS, Guiyang, China between July 2nd and fifth, 2021.

of pure Fe and Fe-alloys in the deep interior of the Earth and other planets (Moon, Mercury, Mars, Ganymede).

Some high-P experimental and theoretical calculating investigations have been reported for some minerals and rocks. Using synchrotron-based single-crystal X-ray diffraction (SCXRD) measurements in a diamond anvil cell, Qin et al. investigated the phase structure of the copper-bearing oxide of cuprite (Cu_2O) up to ~30 GPa and ambient temperature conditions and provide insights into the phase stability and elastic properties of copper oxides and chalcogenides in extreme conditions. Li et al. determined the equations of state of pyrope-almandine garnet solid solutions based on SCXRD experiments at 0–20 GPa and 293–700 K using a diamond anvil cell, outlining that the chemical composition has a crucial influence on the thermoelastic properties of garnet. Sun et al. measured the electrical conductivities of hydrous olivine (Ol) aggregates and Ol–H_2O, Ol–NaCl–H_2O (salinity: 1–21 wt%; fluid fraction: 5.1–20.7 vol%), Ol–KCl–H_2O (salinity: 5 wt%; fluid fraction: 10.9–14.0 vol %) and Ol–$CaCl_2$–H_2O systems (salinity: 5 wt%; fluid fraction: 10.7–13.7 vol%) at 2.0–3.0 GPa and 773–1073 K using a YJ–3000t multi-anvil apparatus. They conclude that the Ol–NaCl–H_2O system with its salinity of ~5 wt% NaCl and fluid fraction larger than 1.8 vol% can account for the high-conductivity anomalies observed in the mantle wedges. Zang and Wang conducted partial melting experiments on the system of garnet plagioamphibolite and 90 wt% garnet plagioamphibolite +10 wt% plagioclase slate mixtures at a temperature range of 1123–1273 K and 1.5 GPa using a piston-cylinder apparatus. They think that the terrigenous sediment made a large contribution to silicic magma generation on both chemical component and melt ratio during the process of partial melting of subducted oceanic crust. Wang et al. performed first-principles theoretical simulations using the density functional theory and obtained the crystalline structure, electrical properties, elasticity, and anisotropy of the observed mantle mineral, CaO_3, within a pressure range of 10–50 GPa. Their results provide further constraints to the compositional and anisotropic issues of the mantle transition zone.

Some acquired theoretical modeling resulting in rock physics parameters are also included in this special topic. An efficient rock physics scheme for the characterization of elastic properties is presented by Jiang et al. The authors applied it to estimate the crack density and fluid saturation of a shale gas reservoir. In the contribution by Wang et al., they conducted molecular dynamic simulations to explore the anisotropic elastic properties of montmorillonite (MMT) with different layer charge densities and layer charge distributions. They think that the density and distribution of layer charges influence the anisotropic elastic properties of MMTs, which may have potential applications to the exploration of unconventional MMT–bearing shale reservoir resources.

In addition, some developments in the high-P instrument and technique are presented in this volume. Ren and Li report on the experimental platform establishment of the six to eight type large-volume high-pressure multi-anvil apparatus in the Key Laboratory of High-temperature and High-pressure Study of the Earth’s Interior, IGCAS. The room-T pressure calibration was completed by using room-T phase transitions of water, ZnTe, ZnS, and GaAs, and its high-pressure calibration was realized with the phase transitions of KCl (850–1,100°C), LiCl (750°C–900°C), KCl + LiCl (450°C–750°C), and SiO_2 (quartz/coesite, 1,000–1,500°C) at high temperature. Yang et al. provided a method for determining geophone orientations based on the zero-offset vertical seismic profile data constrained by a scalar field. In order to check its accuracy, two examples of synthetic and field data were tested, and their results proved that the scalar field method can solve the issue of signal weakness in the first-arrival P-wave well, meaning it is more advantageous than the conventional eigenvalue method.

ETHICS STATEMENT

Written informed consent was obtained from the individual(s) for the publication of any identifiable images or data included in this article.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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