Usage Report for Fiscal Year 2023

Project Title:

Materials properties under extreme conditions: Understanding planets in depth

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1. Background and purpose of the project, relationship of the project with other projects

Metallic state of molten $MgSiO_3$

The electrical conductivity of a planet can provide information on the chemical environment, physical properties and material components inside. Theoretical simulations have been used to understand the electrical conductivity of the Earth. However, most calculations today focus on ionic conductivity. Recently, there has been increasing interest in the possibility of metallization of common prototypical minerals, such as $MgSiO_3$, SiO_2 and MgO, at the conditions of the gas giants, ice giants, and super-Earths. For example, it has been reported that SiO_2 is a poor conductor at 1 TPa and 10000 K. We applied First-Principles Molecular Dynamics (FPMD) calculations to investigate in detail the electrical conductivity of liquid $MgSiO_3$ derived from the melting of bridgmanite as a function of temperature and pressure. While analyzing the electronic structure of $MgSiO_3$ liquids, we noticed the bandgap narrows when the melt was heated to high temperatures at 0 GPa. The observation suggests that the $MgSiO_3$ melt may be a metal at even higher temperatures.

2. Result

Examination of the electronic density of states (DOS) of $MgSiO_3$ different (P, T) conditions (Fig.1) shows the $MgSiO_3$ band gap narrows gradually at 0 GPa. The solid melted at 1600 K, and the band gap of the liquid closed at 4500K, indicating the incipient of a metallic state. At high temperatures, the atoms are diffusive, and the valence electrons can populate the empty states above the Fermi level and liquid metallized at 6000 K at 0 GPa. The electronic density of states (DOS) shows the overlap of the O 2p orbitals is the leading cause of electron conductivity. The partial charge density (within an energy window chosen to be ± 1.4 eV from the Fermi level) of the O linkages at 1600 K and 6000 K were plotted in Fig.2 . At 0 GPa and 1600 K, the interaction between the O lone pair 2p orbitals localized on the atoms and the liquid was non-conducting. When the temperature increased to 6000 K, the lone pair orbitals of O of the polymeric O-O-O linkages overlap significantly, resulting in electron delocalization and a metal.

A comparison of the isosurface partial charge density of liquid melt at different temperatures and 0 GPa within −1.4 eV to +1.4 eV from the Fermi level is more striking (Figure 2). At 300 K and 1600 K, MgSiO3 remains in the glass form. All electrons occupied orbitals with lower energy than the Fermi level, indicating no conducting electrons. When the temperature is increased to 2200 K, the partial charge isosurfaces start to appear, and the electron distribution is metallic-like, meaning that some valence electrons of O have now occupied the empty states above the Fermi level. As the temperature increases, the isosurfaces spread more throughout the system. As was discussed above, the O 2p lone pair orbitals are localized at 1600 K, but at 6000 K the orbitals overlap significantly. This is a significant observation as it indicates that $MgSiO_3$ melt is an electrical conductor at high temperatures, even under ambient pressure.

The electrical conductivity of MgSiO3 liquid was calculated using the Kubo-Greenwood formalism to quantify the metallic character. At each (P,T) condition, the DC conductivity was computed on at least 12 configurations chosen from the equilibrated MD trajectory. Figure 3 shows the average values along with the standard deviations. Note that to estimate the zero frequency conductivity, a Gaussian function of FWHM (dE) is needed to approximate the δ-function (*i.e.* dE $\rightarrow$ 0). The results show at a constant temperature of 6000 K, the electrical conductivity of the melt decreases with increasing pressure. The reason is that at higher pressure, the liquid will solidify at a higher temperature. However, at 140 GPa and 6000 K, the system is still a liquid, as indicated by the calculated diffusion constant.

3. Conclusion

The results from this preliminary study are encouraging. It indicates that when melted, $MgSiO_3$, a principal component of the planet's mineral, can become a metal. This property may have significant implications for the geodynamics and properties of giant planets. Further calculations at even higher temperatures and pressures are underway.

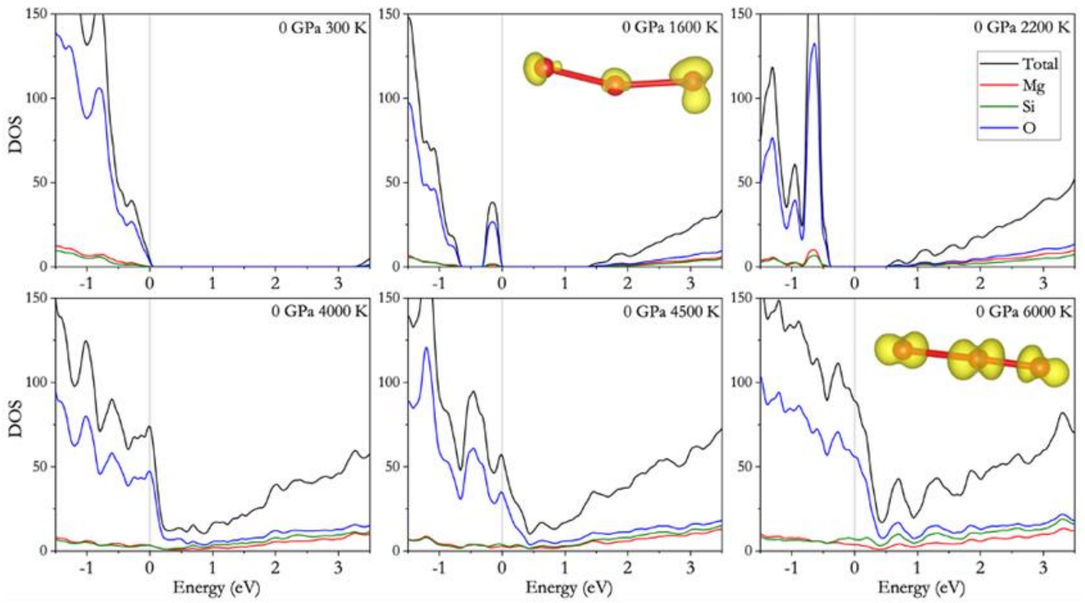
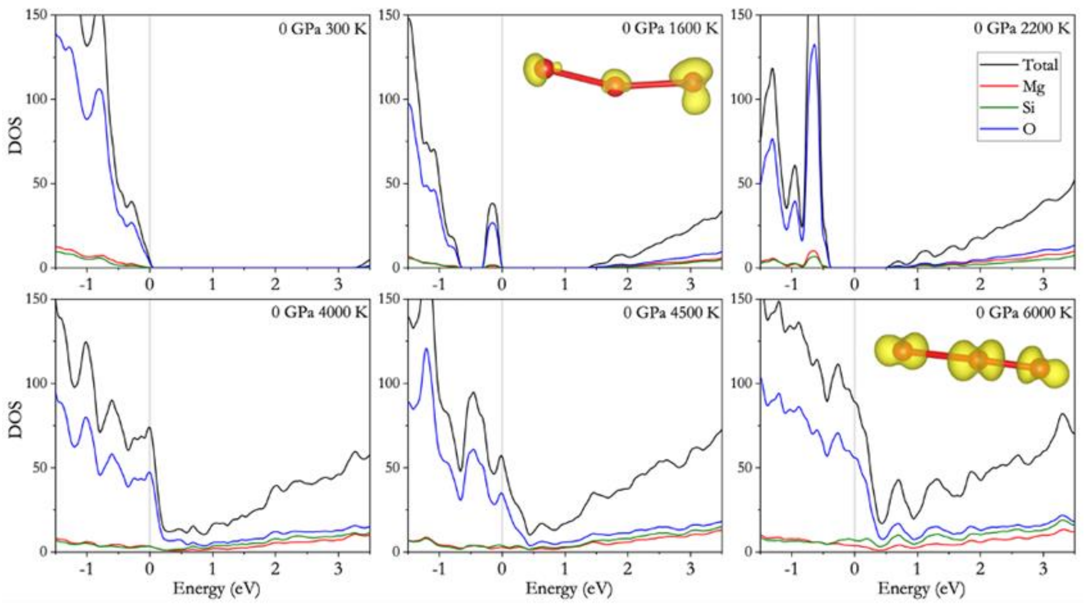


Figure 1. Electronic density of states (DOS) of the constituent atoms in $MgSiO_3$ at different temperatures at 0 GPa. The vertical lines indicate the Fermi level. The insets shown in the 1600 K and 6000 K figures are the partial charge density of O-O-O linkage with the isosurface η = 0.004 at 1600 K and η = 0.012 at 6000 K.



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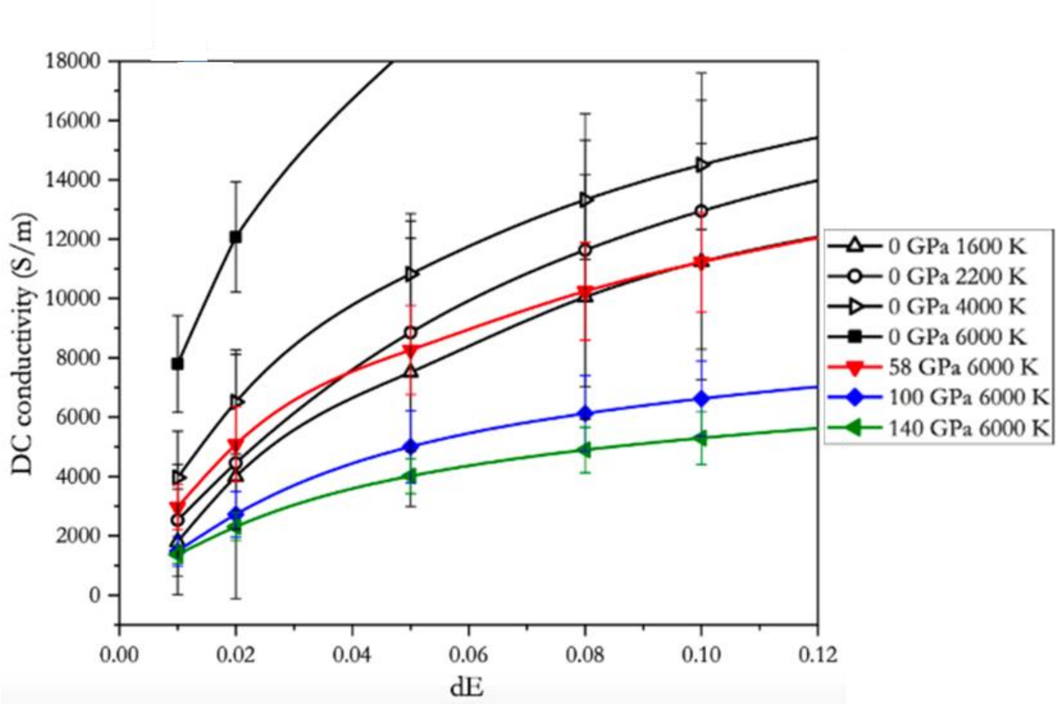

Figure 3. The plot on the top shows the DC conductivity at different (P, T) conditions, from 0 GPa and 1600 K to 140 GPa and 6000 K versus the Gaussian broadening dE.

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