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Density Functional Theory in High Energy Density Physics: phase-diagram and electrical conductivity of water

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Atomistic simulations employing Density Functional Theory (DFT) have recently emerged as a powerful way of increasing our understanding of materials and processes in high energy density physics.

Knowledge of the properties of water (equation of state, electrical conductivity, diffusion, low-energy opacity) is essential for correctly describing the physics of giant planets as well as shock waves in water. Although a qualitative picture of water electrical conductivity has emerged, the necessary quantitative information is scarce over a wide range of temperature and density. Since experiments can only access certain areas of phase space, and often require modeling as a part of the analysis, Quantum Molecular Dynamics simulations play a vital role.

Using finite-temperature density functional theory (FT-DFT), we have investigated the structure and electronic conductivity of water across three phase transitions (molecular liquid/ ionic liquid/ superionic/ electronic liquid). The ionic contribution to the conduction is calculated from proton diffusion and the electronic contribution is calculated using the Kubo-Greenwood formula. The calculations are performed with VASP, a plane-wave pseudo-potential code. There is a rapid transition to ionic conduction at 2000 K and 2 g/cm^3, whereas electronic conduction dominates at temperatures at and above 6000 K[1]. Contrary to earlier results using the Car-Parrinello method[2], we predict that the fluid bordering the superionic phase is conducting above 4000 K and 100 GPa. Our comprehensive use of FT-DFT explains the new findings. The calculated conductivity is compared to experimental data.

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[1] T.R. Mattsson and M.P. Desjarlais, Phys. Rev. Lett. **97**, 017801 (2006).

[2] C. Cavazzoni, et. al. Science **283**, 44 (1999).