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**First principles study of liquid $MgSiO_3$ at conditions of the Earth's deep mantle** JONES TSZ-KAI WAN, Princeton University and The Hong Kong University of Science and Technology, ROBERTO CAR, Princeton University, SANDRO SCANDOLO, The Adbus Salam International Centre for Theoretical Physics and INFM/Democritos National Simulation Center, THOMAS S. DUFFY, Princeton University — Constant-pressure *ab initio* molecular dynamic simulations at high temperatures have been used to study $MgSiO_3$, the major constituent of the Earth's lower Mantle. In this work, we focus the properties of molten $MgSiO_3$, where its existence in the core-mantle boundary is still in debate. By using liquid configuration, we have performed variable-cell *ab initio* molecular dynamic simulations at relevant thermodynamic conditions across one of the measured melting curve. The calculated equilibrium volumes and densities are compared with the simulations using orthorhombic perovskite configuration under the same conditions. For molten $MgSiO_3$, we have determined the diffusion coefficients and shear viscosities at different thermodynamic conditions. Our results provide the evidences of the existence of molten $MgSiO_3$ near the core-mantle boundary.

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