

Abstract Submitted
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Equation of State Calculations of Warm Dense MgSiO₃ FELIPE GONZALEZ¹, HENRY PETERSON, Department of Earth and Planetary Science, University of California, Berkeley, California 94720, USA, FRANCOIS SOUBIRAN, Ecole Normale Supérieure de Lyon, Université Lyon 1, Laboratoire de Géologie de Lyon, CNRS UMR5276, Lyon Cedex 07, 69364, France, BURKHARD MILITZER, Department of Earth and Planetary Science, University of California, Berkeley, California 94720, USA — The equation of state of MgSiO₃ is of significant interest in planetary science and high pressure physics. In order to provide a comprehensive theoretical description of this material at extreme conditions, we combine results from path integral Monte Carlo (PIMC) and density functional molecular dynamics simulation, and generate a consistent equation of state for MgSiO₃. We consider a wide range of temperature and density conditions ranging from 10⁴ to 10⁸ K and 0.1- to 20-fold the ambient density. We derive the shock Hugoniot curve and compare with experimental results. We study how the L and K shell electrons are ionized with increasing temperature and pressure. Finally we analyze the heat capacity and structural properties of the liquid.

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