

Abstract Submitted
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Structural and optical properties of liquid CO₂ up to 1 terapascal¹

BRIAN BOATES, Lawrence Livermore National Laboratory & Dalhousie University, SEBASTIEN HAMEL, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, STANIMIR BONEV, Lawrence Livermore National Laboratory & Dalhousie University — The properties of liquid CO₂ have been studied through first-principles molecular dynamics simulations in the pressure-temperature range of 0-1 TPa and 200-100,000 K. The resulting equation of state data is used to predict shock Hugoniot for several initial conditions. Comparison with available experimental data up to 70 GPa is excellent. We find a gradual phase transition characterized by the destabilization of CO₂ molecules and the formation of other molecular compounds. The liquid phase diagram is divided into several regimes based on a thorough analysis on changes in bonding, structural properties, and chemical composition. Calculations of optical properties such as conductivity and reflectivity will also be discussed.

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