

Abstract Submitted
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First-principles Study of Shock Compressed Carbon NICHOLS

ROMERO, WILLIAM MATTSON, BETSY RICE, U.S. Army Research Laboratory — The phase diagram of carbon at high pressures and temperatures is of scientific interest to material science, geology and astrophysics. Major issues include the liquid-liquid phase transition, the melting curve of graphite and diamond, the nature of the liquid state and the nature of carbon in the interior of Uranus and Neptune. Strong shock waves generated by lasers, and even nuclear explosions have been used to study carbon at these extreme conditions. Because it is often difficult to replicate these shock-wave experiments, first-principles electronic structure calculations can play a prominent role in verifying, guiding, and interpreting these experiments. We report DFT results for the diamond Hugoniot.

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