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Beryllium at high pressure and temperature: A first-principles molecular dynamics study ANDREA TRAVE, ERIC SCHWEGLER, FRANCOIS GYGI, GIULIA GALLI, Lawrence Livermore National Laboratory — *Ab initio* simulations of metals under extreme pressure and temperature conditions are very challenging from a computational standpoint, compared, e.g., to simulations of semiconductors or insulators. Here we present large scale *ab initio* molecular dynamics simulations of a compressed, simple metal at high temperature, beryllium; our calculations are carried out using a two-phase formalism, along with efficient algorithms to determine the electronic ground state at finite temperature, at each ionic step. Our results for the equation of state at 0 K show excellent agreement with previous experiments, indicating that Density Functional Theory can accurately describe the properties of beryllium in the ground state. Melting temperatures as a function of pressure and Hugoniot curves determined from first principles will be presented, and recent shock melting experiments will be interpreted and discussed. This work was performed under the auspices of the US Department of Energy by the University of California at the LLNL under contract no W-7405-Eng-48.

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