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Ab Initio Investigations of High-Pressure Melting of Dense Lithium RAYMOND CLAY, Sandia National Laboratory, MIGUEL MORALES, STANIMIR BONEV, Lawrence Livermore National Laboratory — Lithium at ambient conditions is the simplest alkali metal and exhibits textbook nearly-free electron behavior. As the density is increased, however, significant core/valence overlap leads to surprisingly complex chemistry. We have systematically investigated the phase diagram of lithium at pressures ranging between two and six million atmospheres. Through a combination of density functional theory based path-integral and classical molecular dynamics simulations, we have investigated the impact of both nuclear quantum effects and anharmonicity on the melting line and solid phase boundaries. We also investigate how the inclusion of nuclear quantum effects and approximations in the treatment of electronic exchange-correlation impact the robustness of previous predictions of tetrahedral clustering in dense liquid Li. Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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