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Lithium at ultra-high pressures ANDRE KIETZMANN, RONALD REDMER, Universitat Rostock, Institut fur Physik, D-18051 Rostock, Germany, MICHAEL P. DESJARLAIS, THOMAS R. MATTSSON, Sandia National Laboratories, Albuquerque, NM 87185-1186, USA — Lithium is a prototypical simple metal at standard conditions. However, by changing the density towards expanded or compressed states, the electrical conductivity shows strong variations. We have performed quantum molecular dynamics simulations for fluid lithium covering a wide range of densities and temperatures in order to derive the equation of state, the electrical conductivity, and information about structural and electronic changes along the expansion or compression. The electrical conductivity changes from the nonmetallic expanded fluid via the fluid metal region up to the degenerate electron liquid at high densities. We find a largely ordered ion structure at ultra-high densities reflecting a multi-center bonding situation in the liquid as predicted earlier for solid lithium. Supported by the DFG within SFB 652. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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