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Transport properties of LiF under strong compression: modeling using advanced electronic structure methods and classical molecular dynamics THOMAS R. MATTSSON, REESE JONES, DONALD WARD, CATALIN SPATARU, LUKE SHULENBURGER, Sandia National Laboratories, LORIN X. BENEDICT, Lawrence Livermore National Laboratory — Window materials are ubiquitous in shock physics and with high energy density drivers capable of reaching multi-Mbar pressures the use of LiF is increasing. Velocimetry and temperature measurements of a sample through a window are both influenced by the assumed index of refraction and thermal conductivity, respectively. We report on calculations of index of refraction using the many-body theory GW and thermal ionic conductivity using linear response theory and model potentials. The results are expected to increase the accuracy of a broad range of high-pressure shock- and ramp compression experiments. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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