Many-body Green’s function calculations of optical properties of LiF in extreme conditions\textsuperscript{1} CATALIN D. SPATARU, LUKE SHULENBURGER, Sandia National Labs, LORIN X. BENEDICT, Lawrence Livermore National Labs — We present Density Functional Theory (DFT) + quasiparticle ($G_0W_0$) + Bethe-Salpeter calculations of the real and imaginary parts of the long-wavelength dielectric function of LiF between ambient pressure and \( P = 5 \) Mbars. While the optical absorption spectrum is predicted to show dramatic pressure-dependent features above the optical gap, the index of refraction well below the gap is shown to exhibit the same trends as that seen in both DFT calculations and experiment: a linear increase with \( P \). This increase does not result from a decrease in the band gap, but rather follows from the increase in oscillator strength which counteracts a smaller increase in band gap with \( P \). Our calculations also suggest that the index of refraction (for visible and near-UV light) of the higher-\( T \) B2-phase should be close enough to that of the B1 (ambient crystalline) phase that a transition from B1 to B2 is not likely to present a substantial change in index. These findings may be of interest to researchers who use LiF as a window material in dynamic compression experiments.

\textsuperscript{1}SNL is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Co., for the U.S. DOE’s NNSA under contract DEAC04- 94AL85000. Work at LLNL was performed under the auspices of the U.S. DOE under Contract No. DE-AC52-07NA27344.

Catalin D. Spataru
Sandia National Labs

Date submitted: 14 Nov 2014

Electronic form version 1.4