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Many-body Green's function calculations of optical properties of LiF in extreme conditions[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.

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