Ab Initio Study of the Optical Properties of LiF

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Refractive index n of LiF is investigated using DFT + G_0W_0 + BSE (Bethe-Salpeter equation). We report $n(\omega;\, \rho, T)$ as a function of photon energy ω, density ρ and temperature T.The $n(\rho, T)$ curve is of importance for VISAR and PDV experiments, where n varies with pressure and temperature along the Hugoniot. Our results show the best agreement with experimental data among existing theoretical studies for LiF, supporting the reliability of fully theoretical optical predictions. To obtain accurate n, it is shown that an accurate band gap $(14,2\ eV)$ and excitonic effects are required. The former is obtained with the quasiparticle G_0W_0 method, which captures correlational screening in the Coulomb system. The latter is included via BSE. Excitons reproduce adequate optics for LiF. We show that neither the band gap nor optical absorption is reproduced by the hybrid HSE functional. We account for ionic-temperature effects using QMD and quantify the resulting uncertainty in n, which is novel. The study covers $n(\rho, T)$ up to $P \approx 210\ GPa$. QMD Hugoniot calculations indicate melting near $P \approx 140\ GPa$ under the Lindemann criterion, consistent with studies suggesting melting instead of a B1-B2 transition. Funally, the band gap increases with pressure even until $P \approx 1400\ GPa$, contradicting metallization scenarios proposed so far.

Keywords: LiF; *Ab Initio*; Refractive Index; VISAR; PDV; DFT, QMD, G_0W_0+BSE; Excitons; Ionic Temperature