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The Optical Spectrum of $LaAlO_3$: Quasiparticle Energies and the Effect of Lattice Screening XIAO ZHANG, ANDRE SCHLEIFE, University of Illinois, Urbana — Lanthanum aluminate ($LaAlO_3$) is a commonly used high-κ dielectric material but its exact optical properties are not well understood. By solving the Bethe-Salpeter Equation for the optical polarization function, which describes the interaction between electrons and holes, a precise prediction of the dielectric function can be obtained. However, for $LaAlO_3$, there are two major problems limiting the computational study: The first problem is that due to the complicated conduction band structure, the quasiparticle effect needs to be taken into account, which makes the calculations costly. We resolved this problem by interpolating accurate eigenenergies computed using a hybrid exchange-correlation functional to a dense k-point grid. Another problem is that for such high-κ materials, the lattice contribution to the dielectric screening may be important. We investigated this by computing the optical spectrum using electronic constant, static dielectric constant and the average of both and found that taking lattice contribution into account significantly reduces excitonic effects. All results are compared to available experiments.

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