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First Principles Calculations of Optical properties of PbSe, PbS and the alloy $PbSe_{1-x}S_x$

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Abstract: We have studied the optical properties of the lead chalcogenides PbSe, PbS and $PbSe_{1-x}S_x$ using accurate first principles full potential linearized augmented plane wave method. The (FPLAPW) method was used within the density functional theory (DFT) along with the Generalized gradient approximation (GGA). The refractive index and its variation with the mole fraction are well described. The calculations of linear optical function (refractive index, both imaginary and real parts of the dielectric function, and energy loss) is performed in the photon energy range up to 45 eV. The predicted optical constants agree well with the available previous calculations and experimental measurements. *(30 refs.)*