First principle study: Polaron characteristic & Electron and Hole Mobilities in BiOI

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Bismuth oxyiodides (BiOI) are widely recognized as promising layered materials for photocatalysis and photo-sensing applications due to their cost-effective and environmentally friendly synthesis methods. Unlike many other materials, BiOI can be synthesized without generating toxic byproducts, making them highly attractive for sustainable applications. Typically, BiOI has been investigated through both experimental and theoretical approaches to better understand its optical properties. Given the ionic nature of BiOI, polaron formation naturally occurs within the material. These polarons significantly influence charge transport, yet their characteristics remain relatively unexplored. To examine the formation and nature of polarons in BiOI, we employed density functional perturbation theory (DFPT) and the Fröhlich electron-phonon interaction. The important charge transport input parameters, including effective carrier mass, dielectric constant, and phonon dispersion, were calculated using density functional theory (DFT). Our findings indicate that large polarons preferentially form in BiOI, with electron-phonon coupling constants ranging from 0.79 to 2.49, placing them within the intermediate coupling regime. Notably, the anisotropic properties of BiOI lead to significant variations in the electron-phonon coupling constant, where coupling is weaker in the x-y plane compared to the z-direction. Additionally, the mobility of large polarons was computed and found to align with previous experimental studies. The results suggest that electron mobility in BiOI is higher than hole mobility, primarily due to the lower effective mass of electrons, which allows for freer movement. Therefore, polaronic effects in BiOI must be carefully considered, as they play a crucial role in determining charge transport properties.