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# Simulations of phonon-limited electron mobility in II-VI semiconductors

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Mobility of charge carriers is a physical quantity that determines the performance of semiconductor electronic and optoelectronic devices. It is still a significant challenge to predict its value starting from the crystal structure of the material. To date, such calculations have been performed only for few semiconductor materials, such as Si, GaAs and GaN [1]. In this work, we study the mobility of conduction band electrons in II-VI semiconductors ZnSe, CdTe, ZnTe and CdSe [2].

Temperature dependence of mobility was calculated using an ab-initio methodology, where electronic bands, phonon bands and electron-phonon coupling constants were obtained from density functional theory calculations. Fourier-Wannier interpolation procedure [1] was performed to obtain these quantities on a dense momentum grid which is necessary to obtain reliable values of these quantities. Density functional theory calculations were performed using the ABINIT code, while Fourier-Wannier interpolation was performed using our in-house parallel code.

The results indicated that mobilities obtained from calculations within generalized gradient approximation to density functional theory overestimate the experimental mobility several times. Very good agreement with experiments was obtained when electronic band structure and high-frequency dielectric constants were obtained using the hybrid HSE06 functional [2]. Our results also showed that accurate mobility in these materials can be obtained if we only consider the long-ranged part of electron-phonon interaction, thus avoiding the need for demanding interpolation of electron-phonon coupling constants to a dense momentum grid. We find that even the simple Fröhlich model yields a reasonable estimate of the mobility around room temperature when the dominant scattering mechanism comes from longitudinal optical phonons.

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**References**

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