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

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INTRODUCTION

- Charge carrier mobility of pure crystalline materials is limited by the electron-phonon interaction.
- It is challenging to perform ab-initio prediction of mobility starting from the crystal structure of the material.
- Such studies were performed so far for only few representative semiconductors.
- Further studies are needed to further verify or improve the whole approach for mobility prediction.
- In this work we study II-VI semiconductors: ZnSe, CdTe, ZnTe and CdSe [1].

METHODS

Calculation on the coarse ($\sim 8 \times 8 \times 8$) momentum grid:

- Density functional theory used to obtain the wave functions and energies of electronic states.
- Density functional perturbation theory used to obtain the electron-lattice coupling constants and the phonon modes.

Interpolation to a dense ($\sim 100 \times 100 \times 100$) momentum grid [2]:

- Electronic band structure
  - Construction of unitary matrices that connect the Bloch and the Wannier functions.
  - Representation of the electronic Hamiltonian in the Wannier basis.
  - Diagonalization of this Hamiltonian yields electronic energies at arbitrary electronic wave vector.
- Phonon dispersion / electron-phonon coupling constants
  - Removal of the long-ranged part of dynamical matrices / electron-lattice coupling constants.
  - Transformation of the short-ranged part to force-constant / Wannier representation.
  - Evaluation of the short-ranged part on the dense momentum grid.
  - Putting back the long-ranged part of dynamics matrices / electron-lattice coupling constants.
  - Solving the eigenvalue problem of the dynamical matrices.

MOBILITY

- The mobility is given as (for low electric field and small carrier concentration)

$$\mu_{xx} = e \frac{\sum_{mk} \boldsymbol{v}_{x,mk}^2 \tau_{mk} \frac{\partial f_{mk}}{\partial \varepsilon_{mk}}}{\sum_{mk} f_{mk}}$$

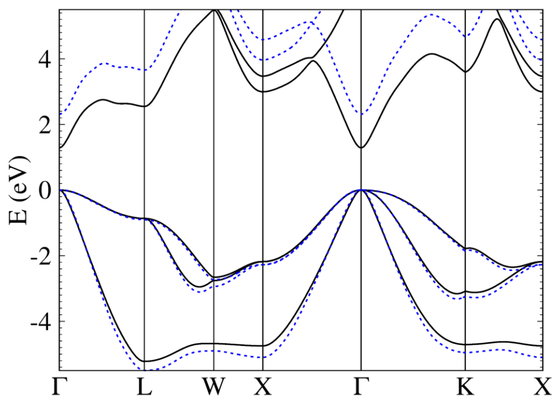
  - f_{mk} is the Fermi Dirac factor
  - $v_{x,mk}$ is the band velocity
  - ε_{mk} is the band energy
  - τ_{mk} is the momentum relaxation time

$$\frac{1}{\tau_{mk}} = \frac{2\pi}{\hbar} \sum_{n\mu q} |\gamma_{nm}^{\mu}(\boldsymbol{k},\boldsymbol{q})|^2 \begin{bmatrix} n_q^{\mu} \delta(\varepsilon_{mk} - \varepsilon_{nk+q} + \hbar\omega_q^{\mu}) + \\ (n_q^{\mu}+1)\delta(\varepsilon_{mk} - \varepsilon_{nk-q} - \hbar\omega_q^{\mu}) \end{bmatrix} (1 - \cos\theta_{k,k\pm q})$$

  - $\gamma_{nm}^{\mu}(\boldsymbol{k},\boldsymbol{q})$ are the e-ph coupling constants
  - n_q^{μ} are the Bose-Einstein factors
  - $\hbar\omega_q^{\mu}$ are the phonon energies

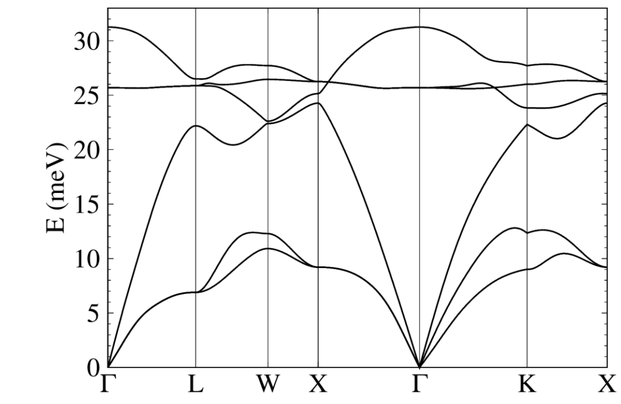
RESULTS

- Electronic band structure of ZnSe obtained using PBE (black) and HSE06 (blue) functional

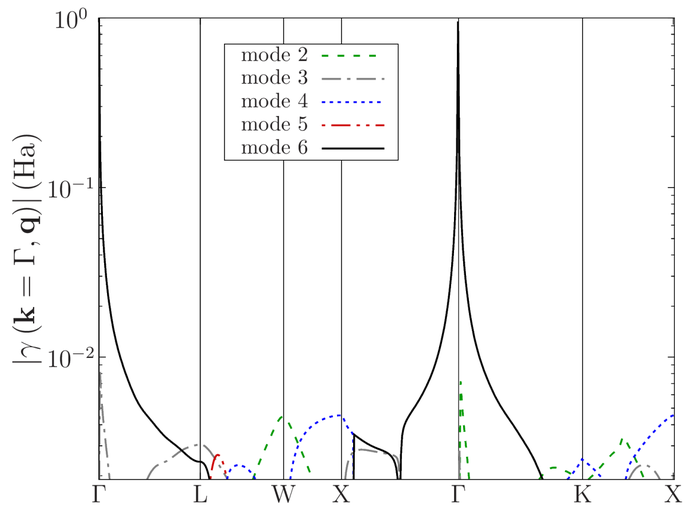


	ZnSe	ZnTe	CdSe	CdTe
m_{eff} exp	0.137	0.117	0.119	0.090
m_{eff} PBE	0.096	0.087	0.061	0.064
m_{eff} HSE	0.14	0.13	0.13	0.13
E_{g} (eV) exp	2.72	2.27	1.68	1.51
E_{g} (eV) PBE	1.29	1.28	0.61	0.77
E_{g} (eV) HSE	2.32	2.19	1.53	1.61

- Phonon band structure of ZnSe

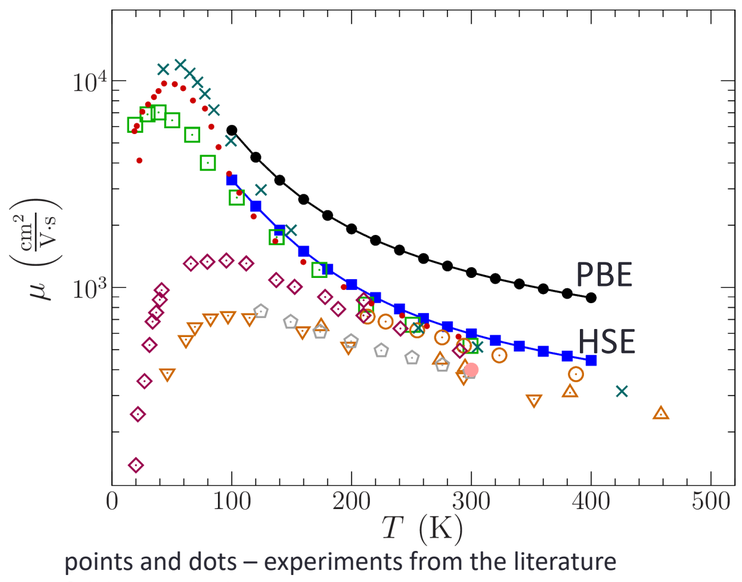


- Electron-phonon coupling constants in ZnSe



MOBILITY - RESULTS

- Temperature dependence of mobility in ZnSe

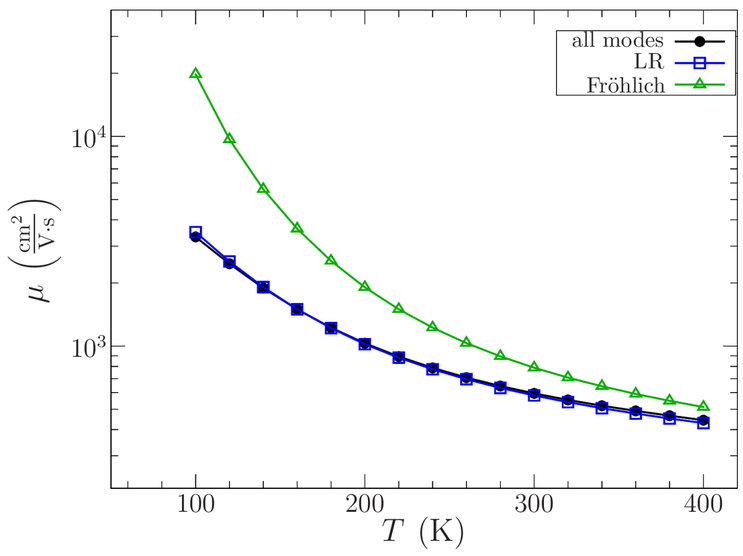


points and dots – experiments from the literature
full line - calculations

- PBE – all calculations with PBE functional
- HSE – band energies and high-frequency dielectric constants from the hybrid HSE functional

	ZnSe	ZnTe	CdSe	CdTe
$\varepsilon_{\text{r}}^{\infty}$ exp	5.9	6.9	6.2	7.1
$\varepsilon_{\text{r}}^{\infty}$ PBE	7.26	8.86	7.72	8.62
$\varepsilon_{\text{r}}^{\infty}$ HSE	6.15	7.45	6.13	7.01

COMPARISON OF DIFFERENT MODELS



	Fröhlich	LR e-ph only	Full calc.
DFT	☑ ☒	☑	☑
DFPT	☒	☑	☑
Interpolation band structure	☒	☑	☑
Interpolation phonon modes	☒	☑	☑
Interpolation e-ph constants	☒	☒	☑
Accuracy	**reasonable at room *T***	**high**	**high**

REFERENCES

[1] N. Vukmirović, Phys. Rev. B 104, 085203 (2021).
[2] F. Giustino et al, Phys. Rev. B 76, 165108 (2007).