Phonon Dispersion by Enhanced Valence Force Field (EVFF)

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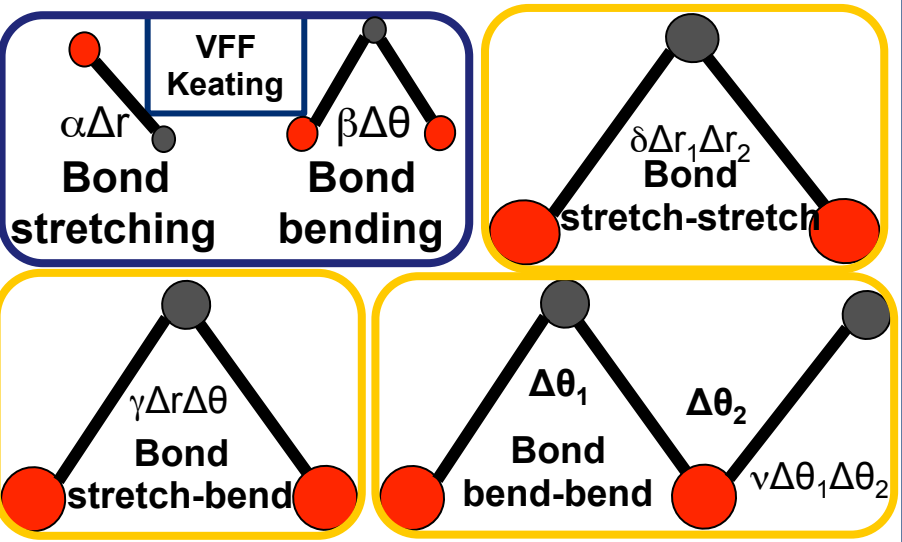
Objective:

- Developing a precise model for calculation of phonon spectra in zinc-blende materials

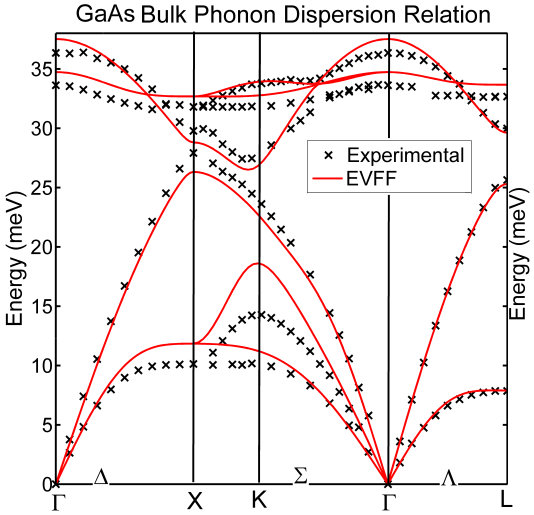
Approach:

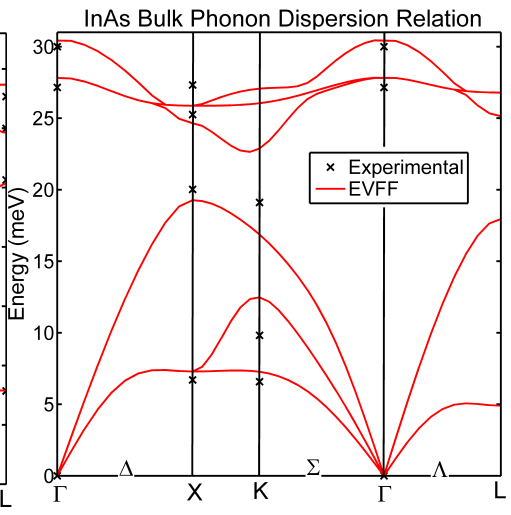


- Plus Coulomb interaction for polar materials
- Parallel genetic algorithm to fit the model's parameters against experimental/*ab intio* phonon spectra

Impact/Results:

- The parameters were fitted for GaAs and InAs bulk
- The model could be well fitted with Experiments





- Parameters table

The parameter sets for InAs and GaAs EVFF model. X could be Ga or As

Param	α	$\beta(X)$	$\beta(As)$	$\gamma(X)$	$\gamma(As)$	$\delta(X)$	$\delta(As)$	ν
GaAs	42.5	7.8	0.01	10.52	-19.98	8.93	-10.55	4.99
InAs	35.03	-0.27	4.13	9.34	-6.24	19.78	-18.49	3.92

1. S. Steiger, M. Salmani-Jelodar, D. Areshkin, A. Paul, T. Kubis, M. Povolotskyi, H. Park, G. Klimeck, "Enhanced valence force field model for the lattice properties of gallium arsenide" *Physical Review B*, Vol. 84, pg. 155204 (2011)
2. M. Salmani-Jelodar, S. Steiger, A. Paul, G. Klimeck, "Parameter Fitting for Lattice Properties of Gallium Arsenide using Parallel Genetic Algorithm" IEEE Congress on Evolutionary Computation (2011)

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