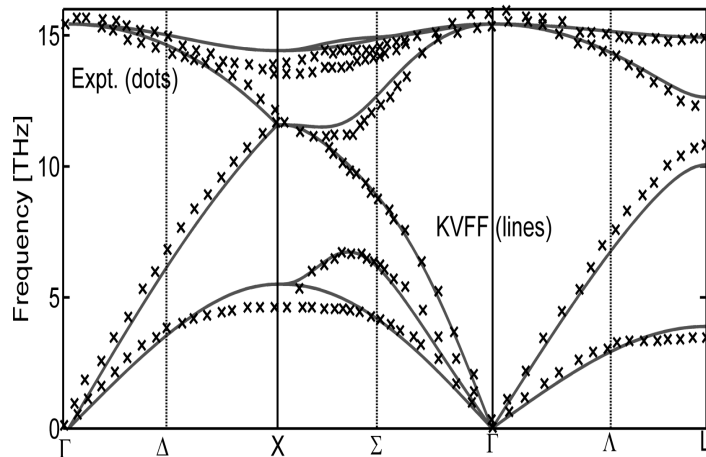


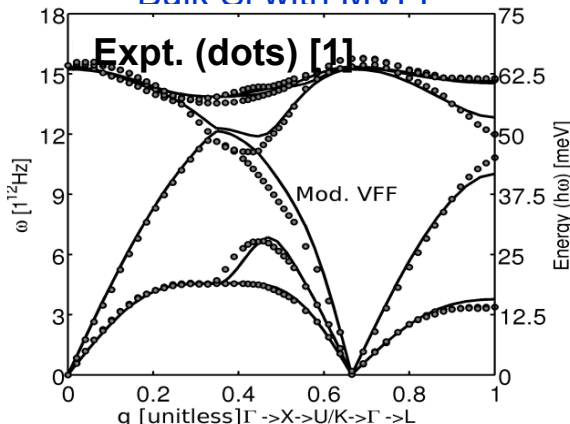
Objective:

- Document phonon parameters in NEMO5.
- Verified parameters of different materials.
- Enable the phonon dispersion calculation in Bandstructure Lab.

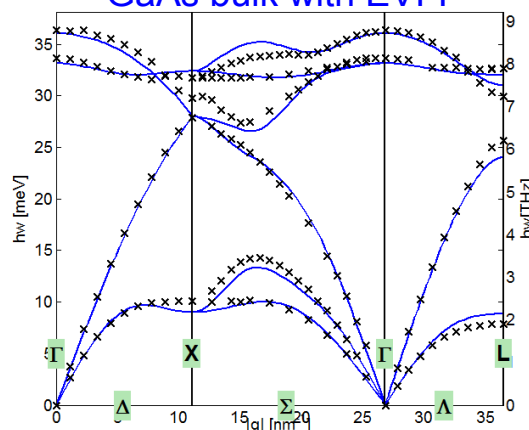
Phonon dispersion documentation: Bulk Si with New Keating parameters



Bulk Si with MVFF

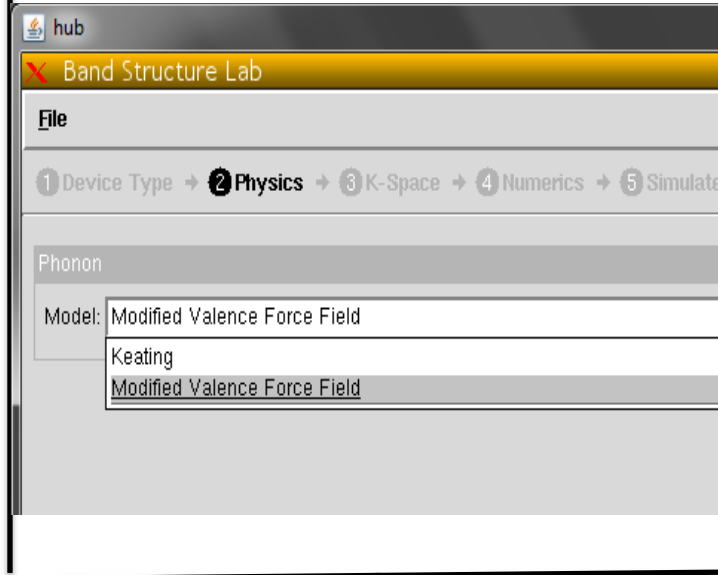


GaAs bulk with EVFF

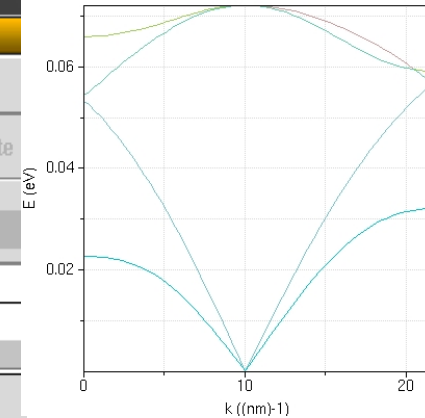


Tool status & Results:

Enable different models in BSL tool.



Bulk Si with MVFF



Impacts:

1. Phonon parameters are well documented in NEMO5.
2. The results in published papers can be reproduced with this tools.