Automated finite temperature calculations in ABINIT with TDEP linked as a library

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Temperature Dependent Effective Potential

By O. Hellman Phys Rev B, 87, 104111.

- Series of tools for finite temperature lattice dynamics
- Temperature dependent phonon frequencies
- **Thermal conductivity**

Not yet implemented in a-TDEP

- **Phonon Lifetimes, Temp Dep elastic constants,** …

Temperature Dependent Effective Potential

By O. Hellman Phys Rev B, 87, 104111.

- Fit DFT forces $\mathbf{F}^{BO}$ by least squares
- Get the 2nd, 3rd, 4th, ... forceconstants

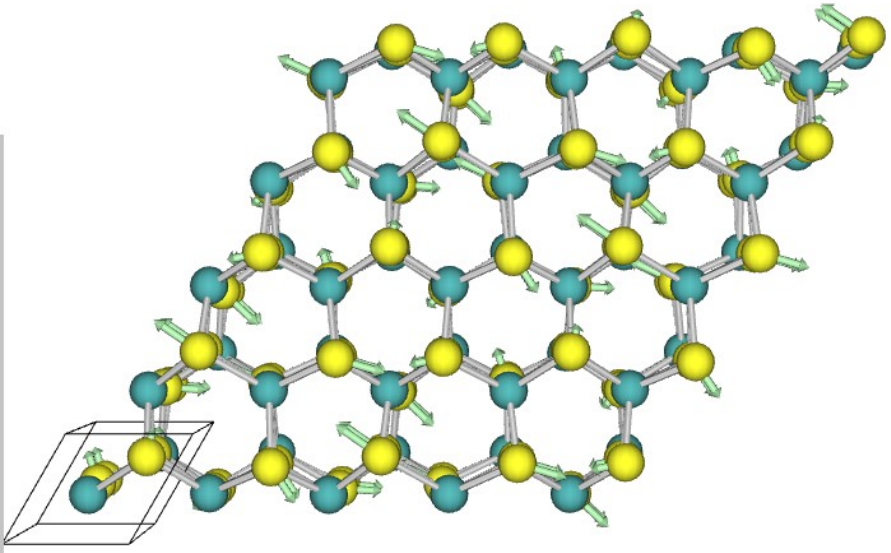
$$min\,\Delta F = \frac{1}{N_c}\sum_{c=1}^{N_c} \left| F_c^{BO} - F_c^{M} \right|^2$$

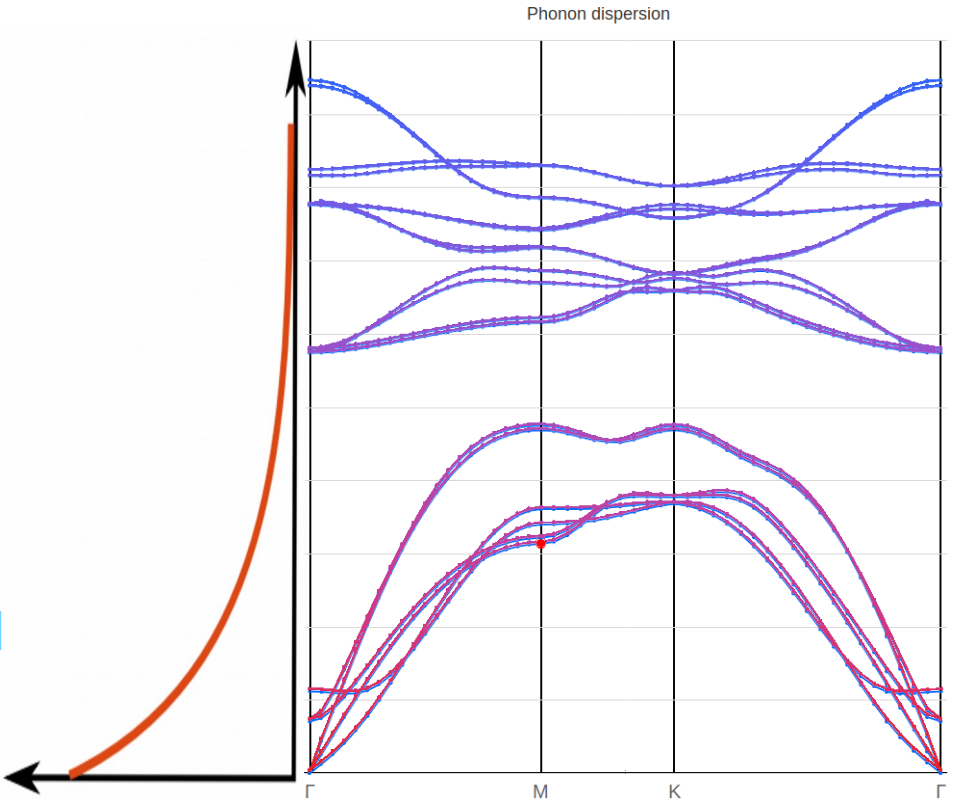
- N_c number of supercell configurations
- F_c^{BO} ab-initio forces of the supercell configurations
- F_c^{M} the forces from an effective model hamiltonian

$$F_{i\alpha}^{M} = -\sum_{j\beta} \Phi_{ij}^{\alpha\beta} u_j^{\beta} - \frac{1}{2}\sum_{jk\beta\gamma} \Phi_{ijk}^{\alpha\beta\gamma} u_j^{\beta} u_k^{\gamma} + \ldots$$

Canonical Configurations

- DFT forces F^{BO} --> Canonical Configurations
- Use (model) forceconstants to generate distorted supercell configurations

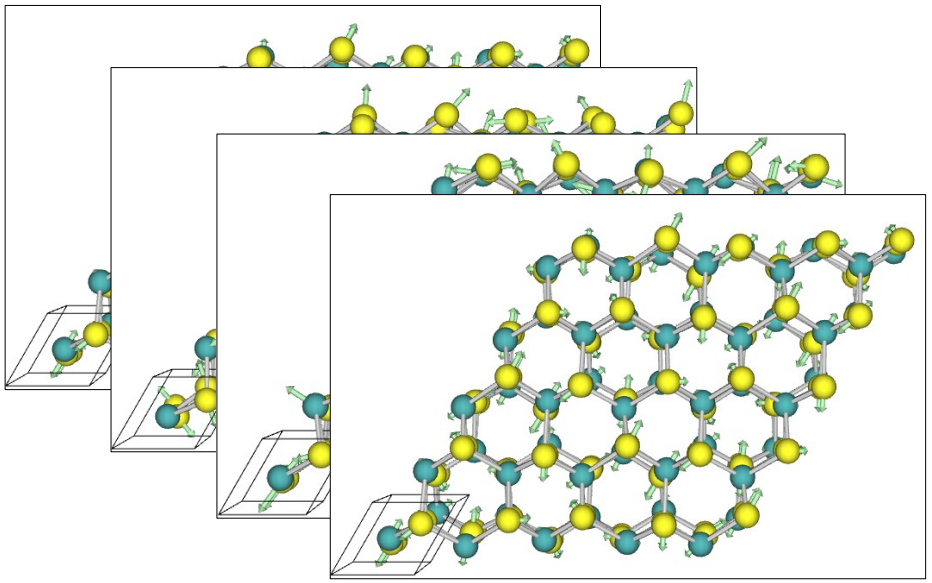




Populating the modes with
a Maxwell-Boltzmann or
Bose Einstein Statistics

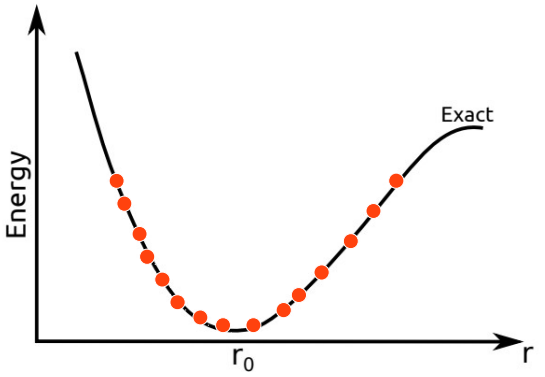
Starting forceconstants do not represent the dynamic at a certain temperature
Need renormalized forceconstant to get correct dynamics

Configurations and convergence



TDEP

Convergence of the fit => paving the phase space of displacement
=> increasing the number of configurations



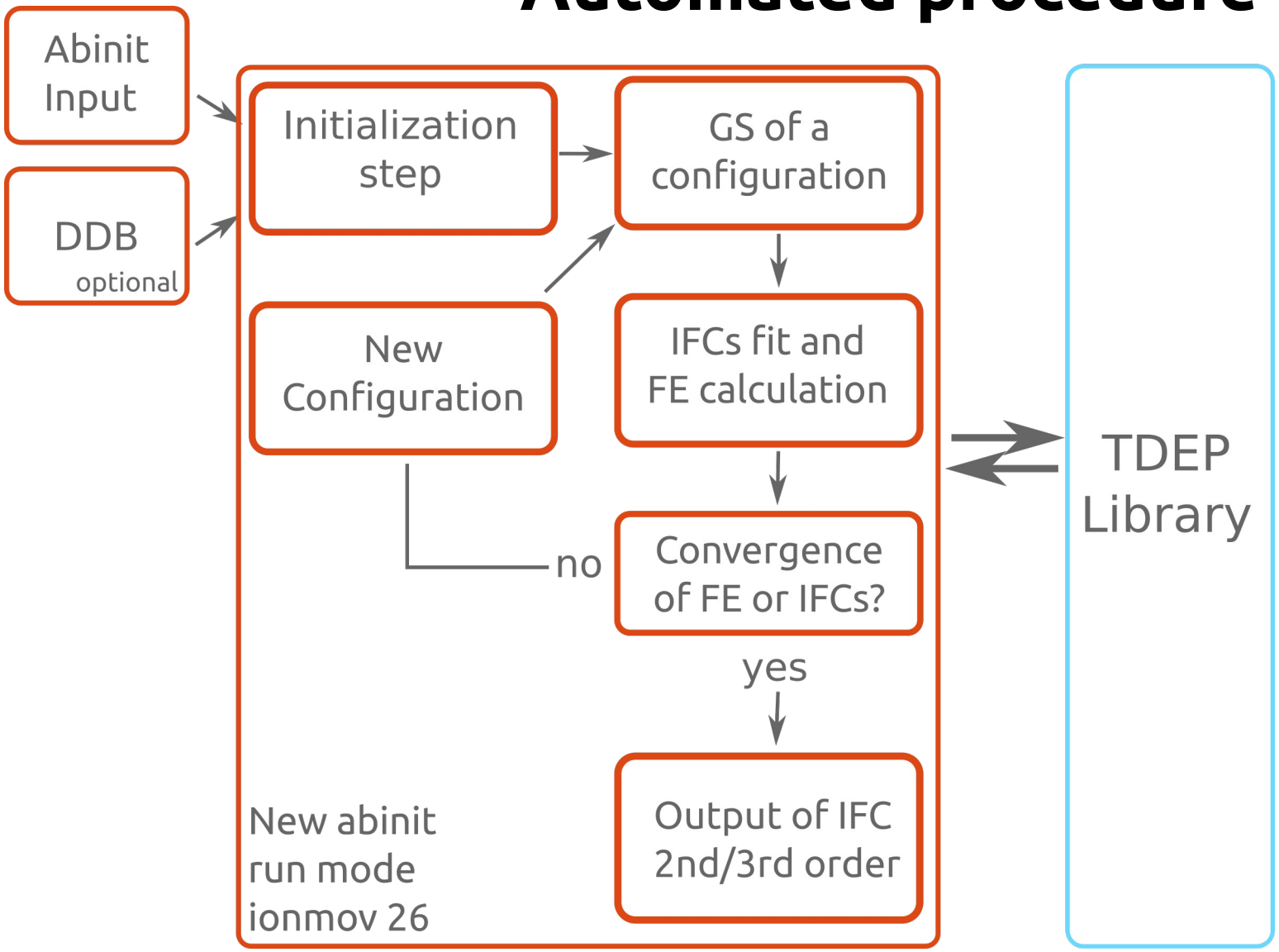
When is it converged
wrt the number of displacement ?

Convergence parameter : Free energy

$$F_{\mathrm{ph}} = \sum_{\lambda} \frac{\hbar\omega_\lambda}{2} + k_B T \ln\left(1 - \exp\left(-\frac{\hbar\omega_\lambda}{k_B T}\right)\right)$$

Interface ABINIT/TDEP

Automated procedure



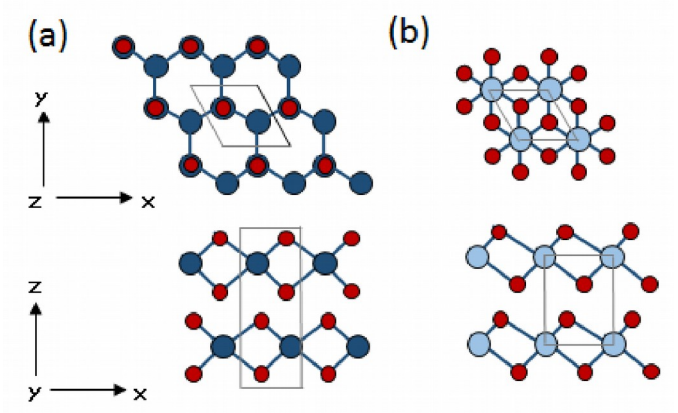
TDEP is implemented as a library

Abinit calls the TDEP subroutines

$NbSe_2$ Application

And why it is important to update the input forceconstant

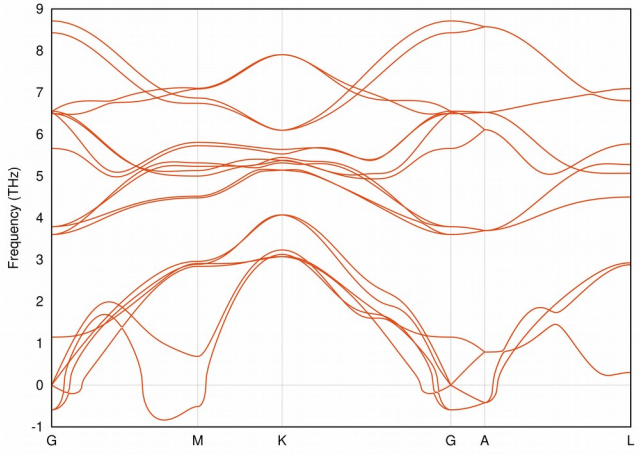
$NbSe_2$: TMD materials with a Charge Density Wave



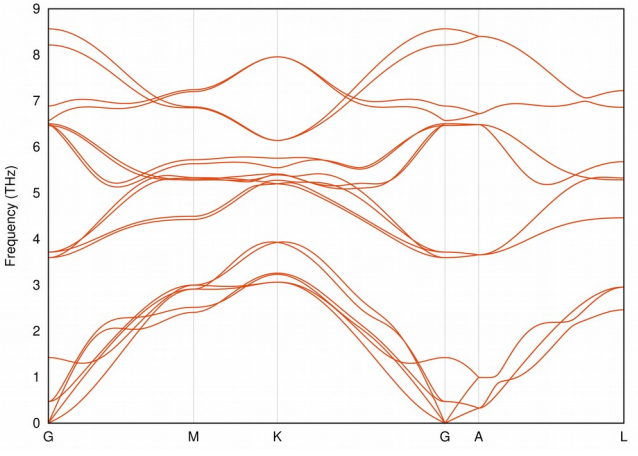
Unstable at 0K

Hexagonal structure stabilizes with temperature

Starting from debye model
WITHOUT updating



Starting from DFPT
Updating at each step



Conclusion

Thank for you attention!