

Interatomic force constants  
and  
phonon dispersion

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## Real-space interatomic force constants (IFCs)

$$C_{st}^{ab}(\mathbf{R}) = \frac{\partial^2 E}{\partial u_s^a(\mathbf{0}) \partial u_t^b(\mathbf{R})} = \frac{1}{N_c} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}} \tilde{C}_{st}^{ab}(\mathbf{q})$$

- Calculation of  $C_{st}^{ab}(\mathbf{q})$  on a suitable grid of  $\mathbf{q}$ -vectors
- Fourier transform to real space

## Real space interatomic force constants

The *shorter* the range of real-space IFCs, the *coarser* will be the reciprocal-space grid needed for the Fourier transform. The size of the grid is assessed *a posteriori* by verifying that it yields vanishing real-space constants beyond a certain cutoff radius.

For **non polar systems**, the IFCs are relatively short range, thus requiring a moderate number of calculations at different  $\mathbf{q}$ .

For **polar systems**, the IFCs are long ranged. But Fourier interpolation is efficiently applicable to the *analytic* contribution to IFC, while the *nonanalytic* behavior is restored by adding the IFC of a suitable point charge model.

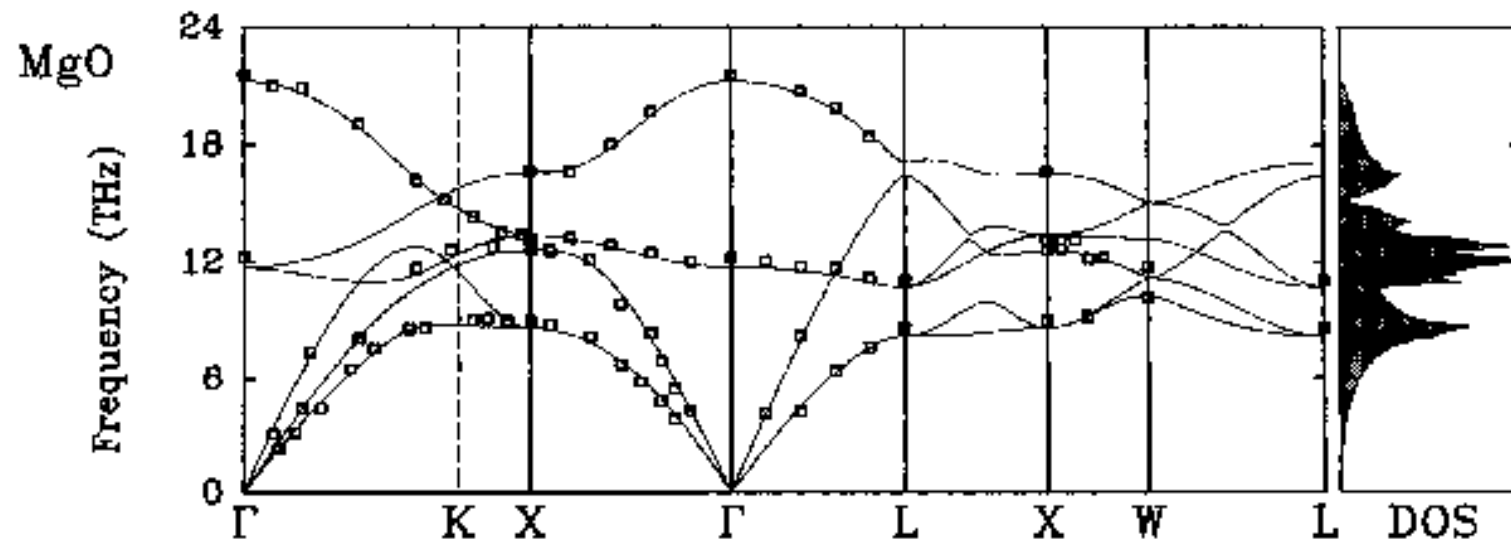
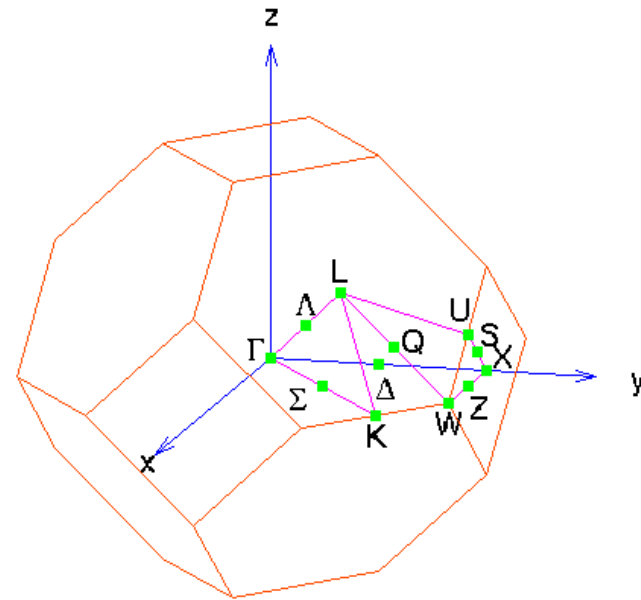
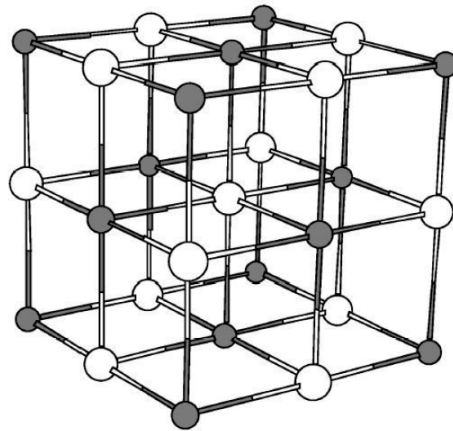
# Phonon dispersion

Once real-space IFCs have been computed, dynamical matrices in reciprocal space (and, hence, vibrational frequencies) can be obtained at any wave vector (*not necessarily contained in the original grid*) by Fourier transform.

$$\tilde{C}_{st}^{ab}(\mathbf{q}) = \sum_{\mathbf{R}} e^{-i\mathbf{q}\cdot\mathbf{R}} C_{st}^{ab}(\mathbf{R})$$

The comparison of the results of this procedure with the full calculation on some points *not* included in the original grid (used to compute the IFCs) is a check of the accuracy of the Fourier interpolation .

# Phonon dispersion of MgO



# Phonon dispersion of MgO

- Calculation of  $C_{st}^{ab}(\mathbf{q})$  on a 4 x 4 x 4 grid ---> ph.x
- Calculation of the real-space IFCs ---> q2r.x
- Calculation of the phonon dispersion ---> matdyn.x
- Calculation of the vibrational density of states ---> matdyn.x