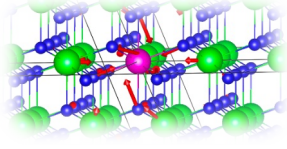


# Lineshape (multi-phonon)

- $E_{\text{ZPL}}$
- $\Delta R_{\kappa\alpha}$  or  $\Delta F_{\kappa\alpha}$   
(obtained from  $\Delta\text{SCF}$  post-process block)



$\Gamma$  q-point phonons  $(\omega_\nu, \mathbf{e}_{\kappa,\nu})$   
(from embedded IFCs block or not)

phonopy object

- Semi-automatic structure mapping
- Huang-Rhys spectral function  $S(\hbar\omega)$
- Phonon mode localization
- Temperature dependent PL spectra following generating function

