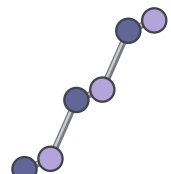


Relaxed Structure

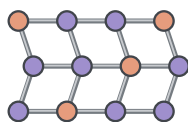
0D, Molecule



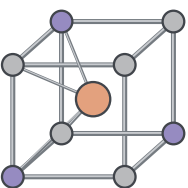
1D, Nanowire



2D, Slab



3D, Bulk

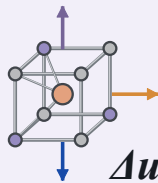


dim = 0 / 1 / 2 / 3

Automated Workflow

Symmetry-Adapted Finite-Displacement

Reduction of calculations by symmetry operations



Reference SCF Calculation

Insulating check, charge density reference

ABACUS + PYATB

Polarization, forces, optical response

Polarization & Dipole

Periodic: Berry phase
Non-periodic: cube integration



Force Difference



Multi-Scheduler Workflow Automation
Agent Skill Support

Unified Calculations

Joint Reconstruction

Polarization multi-branch matching
Symmetry completion: atoms + directions
Joint fit: BEC + force constants

Born Effective Charges

$$\mathbf{Z}_{\kappa}^* = \frac{\Omega}{e} \frac{\partial \mathbf{P}}{\partial \mathbf{u}_{\kappa}}$$

$$\begin{bmatrix} Z_{xx}^* & Z_{xy}^* & Z_{xz}^* \\ Z_{yx}^* & Z_{yy}^* & Z_{yz}^* \\ Z_{zx}^* & Z_{zy}^* & Z_{zz}^* \end{bmatrix}$$

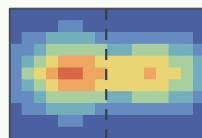
Zone-Center Phonons

$$\Phi_{\kappa'\kappa}^{\Gamma} = - \frac{\partial \mathbf{F}_{\kappa'}}{\partial \mathbf{u}_{\kappa}}$$

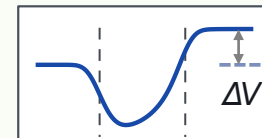
Phonon Modes
Irreps Classification



Polarization in 2D Materials



In-plane polarization potential map



Out-of-plane polarization potential profile

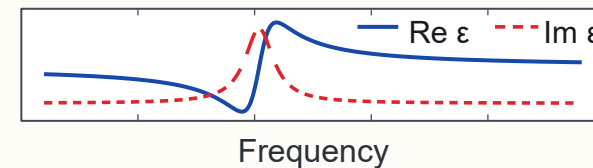
Dielectric and Spectroscopy

Static Dielectric Function

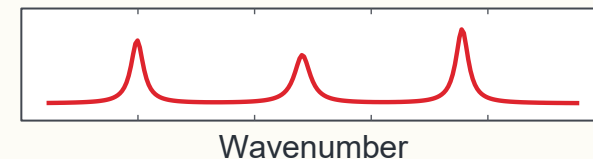
$$\epsilon(0) = \epsilon^{\infty} + \epsilon^{\text{ph}}(0)$$

Electronic + Phonon contributions

Frequency-Dependent Response



Infrared Spectra



Raman Spectra

