



ZStar

Unified finite-displacement response framework

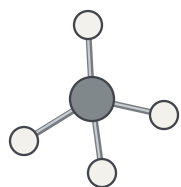
—> Solid: response workflow

- - -> Dashed: optional inputs

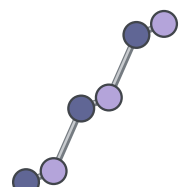
A, B: matching data ports

Relaxed structure

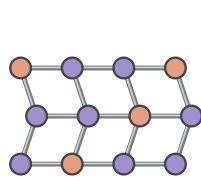
0D, Molecule



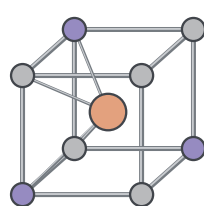
1D, Nanowire



2D, Slab



3D, Bulk

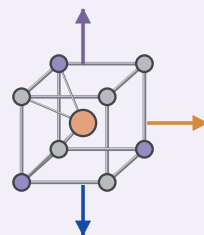


dim = 0 / 1 / 2 / 3

Unified calculation

Symmetry-adapted displacements

Phonopy symmetry seeds
Actual displacement vectors
zstar bec pre --stru STRU



Reference first: 0.no-move

SCF → band-gap check
Private copies of reference density

ABACUS + PYATB

One symmetry-adapted SCF ensemble
zstar bec run

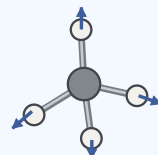
Polarization / dipole changes

Periodic: Berry phase
Open: cube integration



Force changes

$F(d) - F(0)$



Electronic response

Same SCF matrices

Response data

Joint reconstruction

Branch matching + site symmetry
 $Y_K \approx B_K X_K$ rank $X_K = 3$
Raw tensors + sum-rule projections
zstar bec / spectra post

Unified response data

response.json

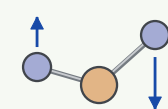
BEC / molecular APT

BEC.dat + BORN

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

Γ -point phonons

FORCE_CONSTANTS
Modes + symmetry labels



Electronic response

Dielectric + its derivatives



Compatible external data

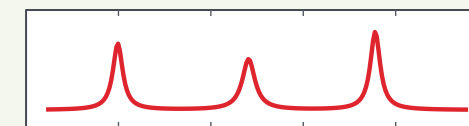
VASP · CP2K · Quantum ESPRESSO
Independent Phonopy calculations

Backend-dependent capabilities
Finite-q phonons: supercell workflow

Analysis and outputs

Infrared spectra

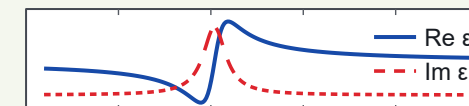
Mode charges + oscillator strengths
zstar spectra



Frequency

Dielectric response

Static / frequency / optical
zstar dielectric



Frequency

Symmetry + mode projection

Same-displacement response
No additional SCFs

Raman tensors

Raman spectra

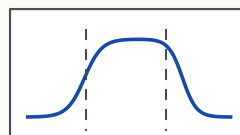
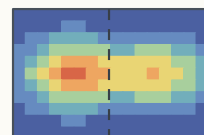
zstar spectra



Frequency

Electrostatic potential: zstar pot

Potential maps, profiles and vacuum steps



Workflow control: pre / job / run / stat / post

Shell / Slurm / Torque

zstar config

Agent Skill: run-zstar-workflows

Dimension-aware response conventions