

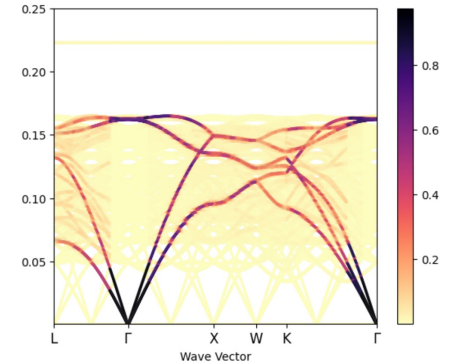
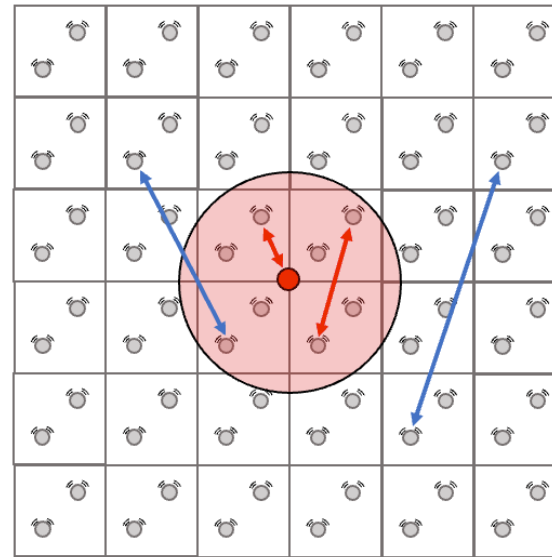
Abipy/dfpt/converters.py

- folding procedure
- DDB \leftrightarrow phonopy format

Abipy/embedding/embedding_ifc.py

IFCs embedding

- Semi-automatic structure mapping
- Creation of embedded IFCs
- Enforcing ASR



Defect phonons
in large supercell

DDB or
phonopy
object

phonopy
object

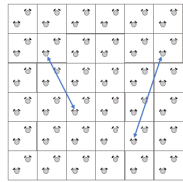
DDB or
phonopy
object

phonopy object

Pristine
phonons
(dense \mathbf{q} -grid)



Folded
pristine
phonons
(Γ \mathbf{q} -point)



Defect
phonons
(Γ \mathbf{q} -point)

