

Abipy/dfpt/converters.py

- folding procedure
- DDB \leftrightarrow phonopy format

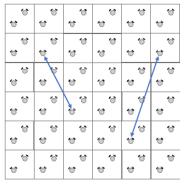
DDB or
phonopy
object

phonopy
object

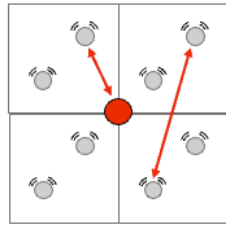
Pristine
phonons
(dense q -grid)



Folded
pristine
phonons
(Γ q -point)



Defect phonons
(Γ q -point)

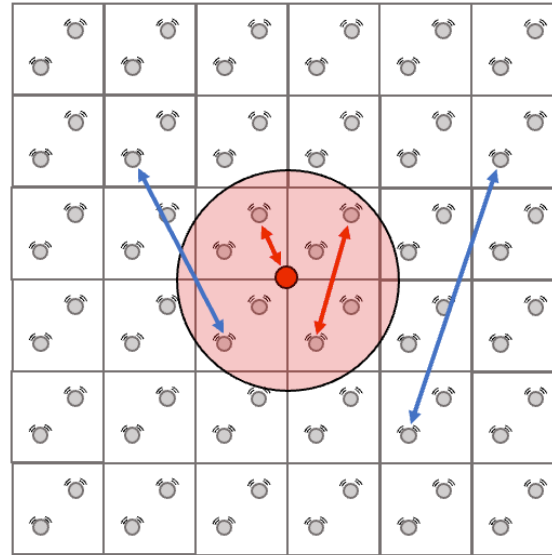


phonopy
object

Abipy/embedding/embedding_ifc.py

IFCs embedding

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



DDB or
phonopy
object

Defect phonons
in large supercell

