

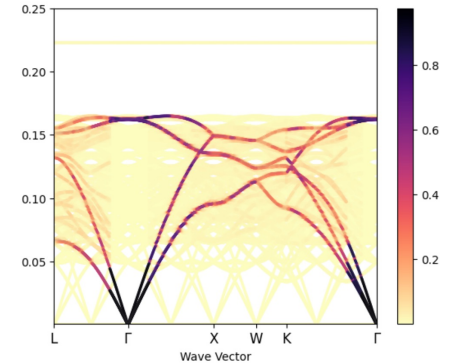
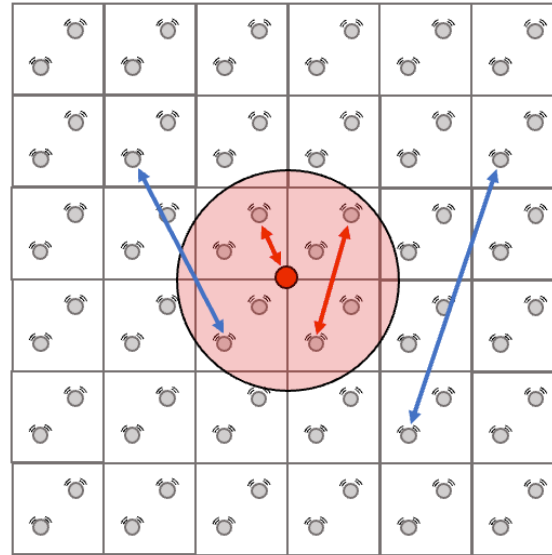
Abipy/dfpt/converters.py

- 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

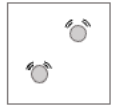
DDB or  
phonopy  
object

phonopy  
object

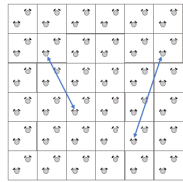
DDB or  
phonopy  
object

phonopy object

Pristine  
phonons  
(dense q-grid)



Folded  
pristine  
phonons  
( $\Gamma$  q-point)



Defect  
phonons  
( $\Gamma$  q-point)

