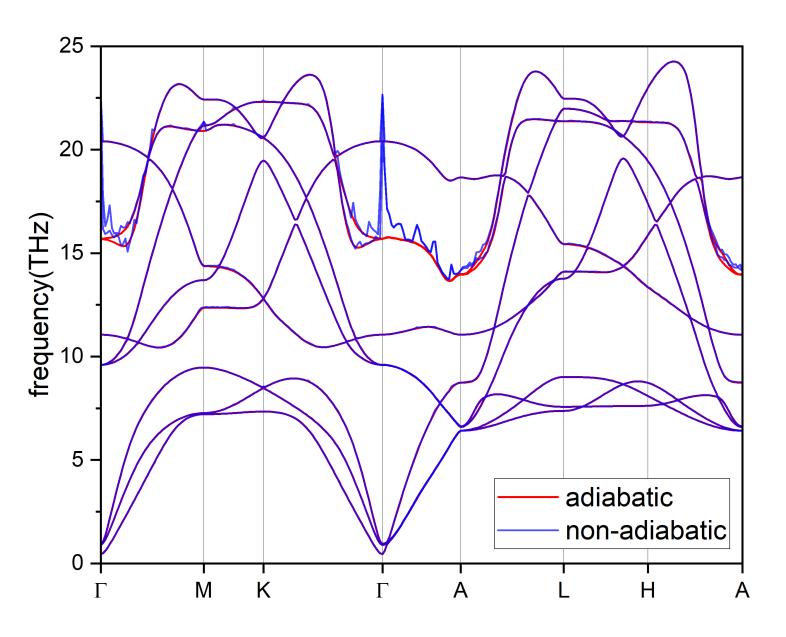


input file from
epiq-EPIq-1.1/tutorials/mgb2/input\_examples

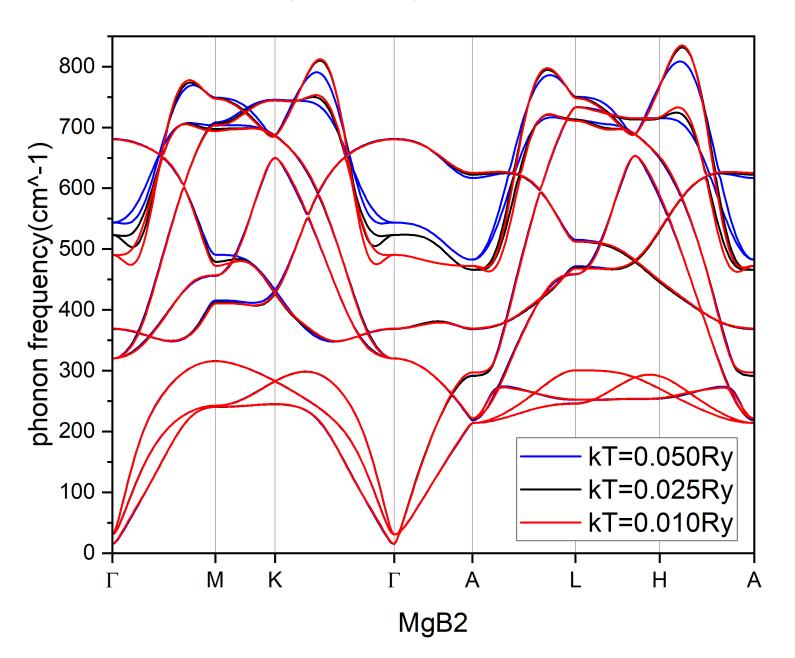
q-points 6x6x4 asr: no

SCF calculation:
k-points 16x16x12
ecutwfc=35
smearing=methfessel-paxton
degauss=0.025
functional PBE
Pseudopotential from tutorials



broad\_min=0.0005 q-points 6x6x4 asr: no k-points 24x24x18 Ecutwfc=50 smearing=methfessel-paxton degauss=0.025 functional PBE Pseudopotential from tutorials

## adiabatic phonon frequencies for different T



k-points:

0.050 16x16x12

0.025 24x24x18

0.010 28x28x21