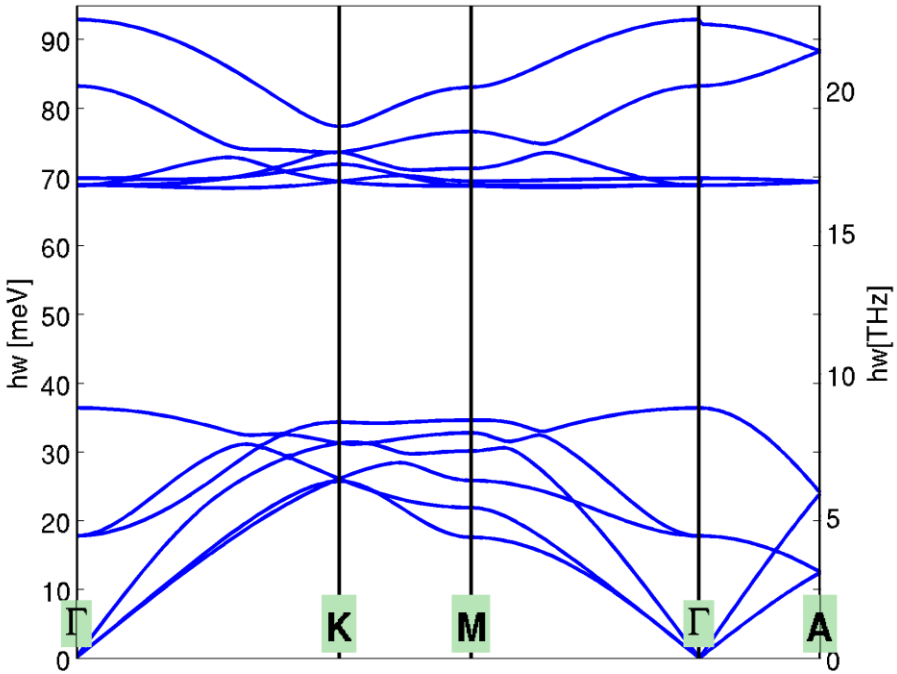
Phonon Simulations in NEMO 5

- Objective:
  - » Calculate phonons in bulk and nanostructures using atomistic valence-force-field (VFF) models
  - » Zincblende or Wurtzite lattices
  - » Coulomb interaction is important for optical branches

- Approach:
  - » Recycle 2nd derivative of VFF strain calculation for dynamical matrix → same physics
  - » Include Coulomb interaction using Ewald summation
  - » Do genetic algorithm fitting to find parameters (with M. Salmani)

- Results / Impact:
  - » Models easily switchable in input deck
  - » Improved anharmonic model: both physical validity and numerical convergence



Bulk phonon dispersion for GaN in wurtzite phase calculated using Keating VFF + Coulomb