Atomic Structure of QD's - procedure and consequences

- **Aim**
  - » To study the effect of the two strain models in NEMO3D on the atomic and electronic structure of pure InAs/ GaAs QD's.
- **Procedure**
  - » Set up device in NEMO3D
  - » Set lattice constant of structure = lattice constant of GaAs.
  - » Minimize total strain energy w.r.t each atomic position ➔ find relaxed atomic positions (R_i)
  - » Set up Tight Binding Hamiltonian using bulk params. and (R_i) and solve Schrödinger equation
  - » Repeat for anharmonic strain model.
- **Result**
  - » Both strain models →InAs is only compressively strained. (-1 to -5%)
  - » Strain in Anharmonic model < Strain in harmonic model.