Internal Fields in InAs/GaAs QDs (Crystal Symmetry, Strain, and Piezoelectricity)

Objective:

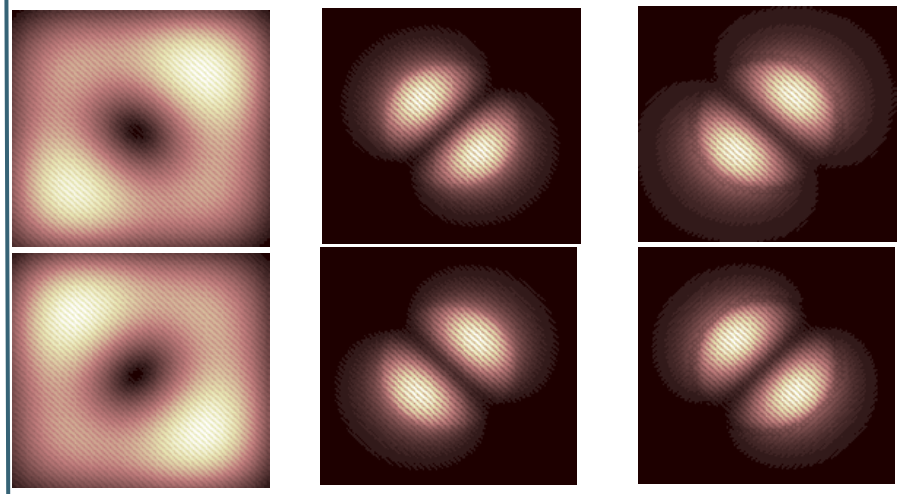
- To investigate the competing effects of various internal/built-in fields on the electronic structure of realistically- sized InAs/GaAs quantum dots.

Approach:

- Use fully atomistic NEMO 3-D simulator
- Include piezoelectric charges through electrostatic potential that goes into the diagonal of the Hamiltonian
- Compare the effects of
  - Crystal and interfacial atomicity
  - Strain
  - Piezoelectricity

Impact:

- Demonstrated quantitative agreement with experiment
- Atomistic approach is essential



no strain | with strain | w/ strain&piezo

Result:

- Disk shaped dots d=10nm, h=2.5 nm, 10nm cap, 20nm substr., 0.6nm WL
- Crystal symmetry alone breaks symmetry of set of first excited states (weak)
  => effective mass, k.p fail!
- Strain further breaks symmetry
- Piezoelectric effect opposes strain
  => can flip the orientation of the excited states