

Objective:

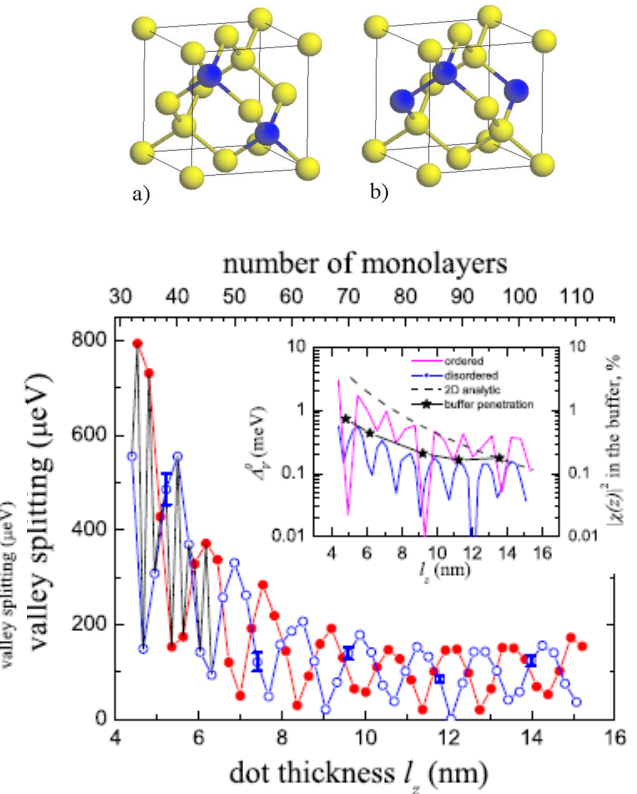
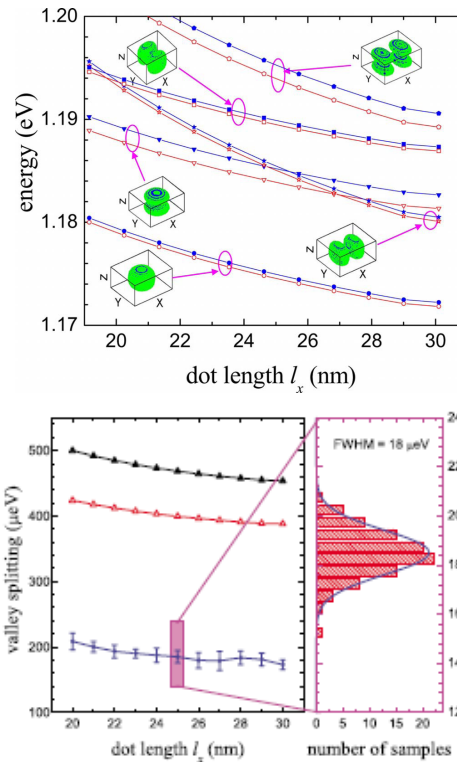
- Obtain energy levels and valley-splitting trends of strained Si quantum dots embedded in $\text{Si}_{0.75}\text{Ge}_{0.25}$ for dimensions relevant to qubit implementation.

Approach:

- Use NEMO 3-D
- Strain Relaxation: VFF Keating.
- Incorporated different levels/orientations of buffer disorder.
- Typical dimensions: $L_x=25\text{nm}$, $L_y=20\text{nm}$, $L_z \sim 10\text{nm}$. 80nm^3 buffer.

Impact:

- Atomistic approach is essential
- Comprehensive study of Si-QDs that provides a reliable benchmark for experimentalists.



Result:

- Valley splitting depends on the wavefunction fraction penetrating into the buffer.
- Valley splitting is suppressed as buffer disorder increases.
- Valley splitting is unaffected by strain.