Geometry Morphology of 1 nm nanowires

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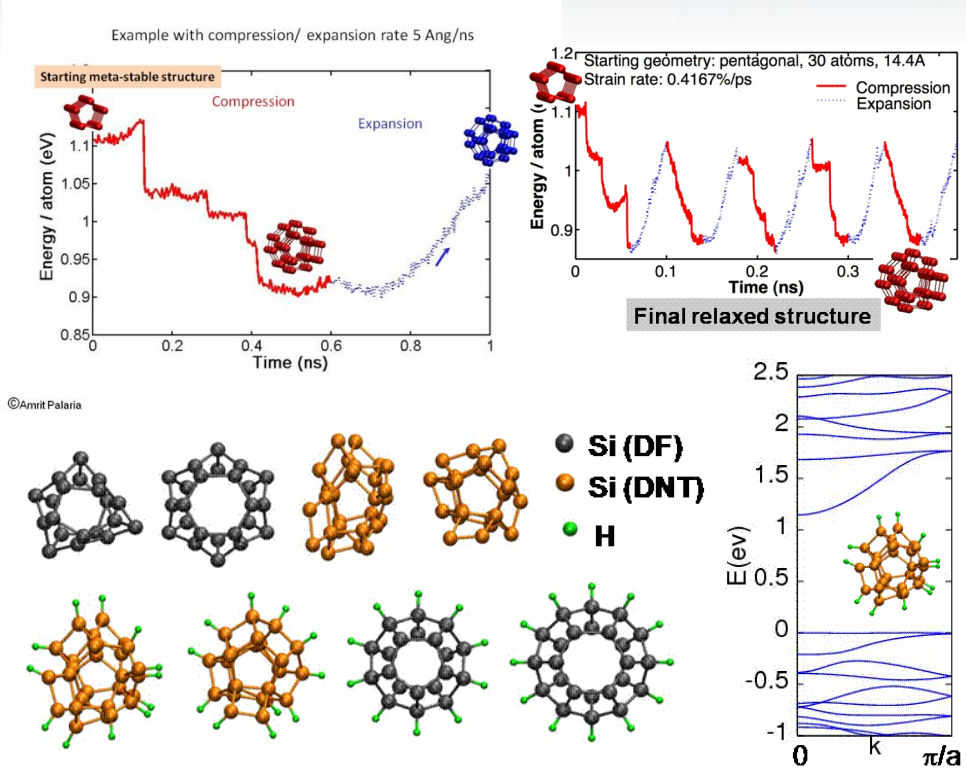
***Objective*:** Investigate the structures and properties of ~1nm dia 1-D silicon nano structures

***Method*:** Density functional theory, reactive force field molecular dynamics

Results:

- 2 categories of **energetically most stable** Si nanowires (NW) of dia ~ 1nm
- Stable wires possess **non-diamond geometries**
- **Structural symmetry reduction** at wire surface enhances stability and introduces bandgap
- **Pristine and H passivated** wires with new bandgaps and **unique properties**



Impact:

- New materials: energy conversion devices, sensors, CMOS scaling
- General method for exploration of new materials