Tight binding parameters for silicon surface

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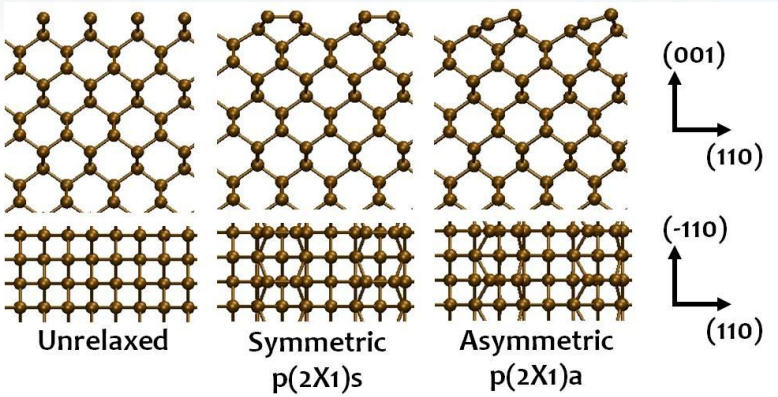
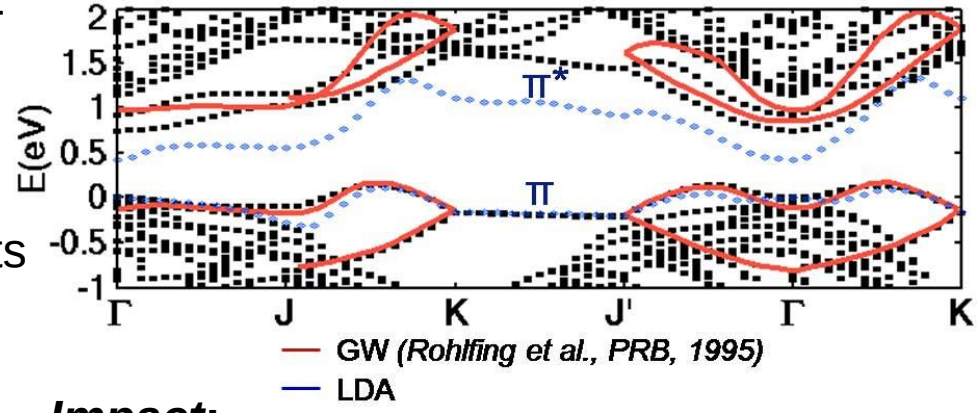
Objective: Investigate the possibility of simulating surfaces and interfaces with empirical tight binding

Method:

- Investigate $sp^3d^5s^*$ tight binding using bulk with strain parameters for Si slab with (100) surface, modify NEMO-3D for this (in C++)
- Use GW results as benchmark
- Modify surface atom bulk parameters
- Check sensitivity of high symmetry points to bulk parameter modification





Result:

- Band-structure of Si(100) surface from TB with modified sigma parameters matches reasonably with GW results

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Impact:

- Quick and scalable simulation of realistic electronic devices with surfaces or other non-bulk bonds e.g. interfaces