

Motivation:

- Uniaxial $\langle 110 \rangle$ strained Si increases mobility
- Lack of good tight-binding(TB) model

Objective:

- Developing a tight binding model for uniaxial strained Si in $\langle 110 \rangle$

Approach:

- Achieving affected on-site energies and coupling between different on-site orbitals
- Optimization method for fitting parameters (Genetic Algorithm with Least Square)
- Van de Walle's model for band edges energies and VASP for effective masses
- Considering model behavior in real device

Result:

- less than 5% disagreement with experimental results in wanted range ($\pm 1.5\%$ strain)

Impact:

- Working well for uniaxial $\langle 110 \rangle$ and $\langle 001 \rangle$ and hydrostatic strain

Results

