Mapping of ab-initio to Tight Binding

Motivation:

Extract TB parameters from DFT results (DFT energy bands & eigenfunctions)

Approach:

- Low rank approximation:

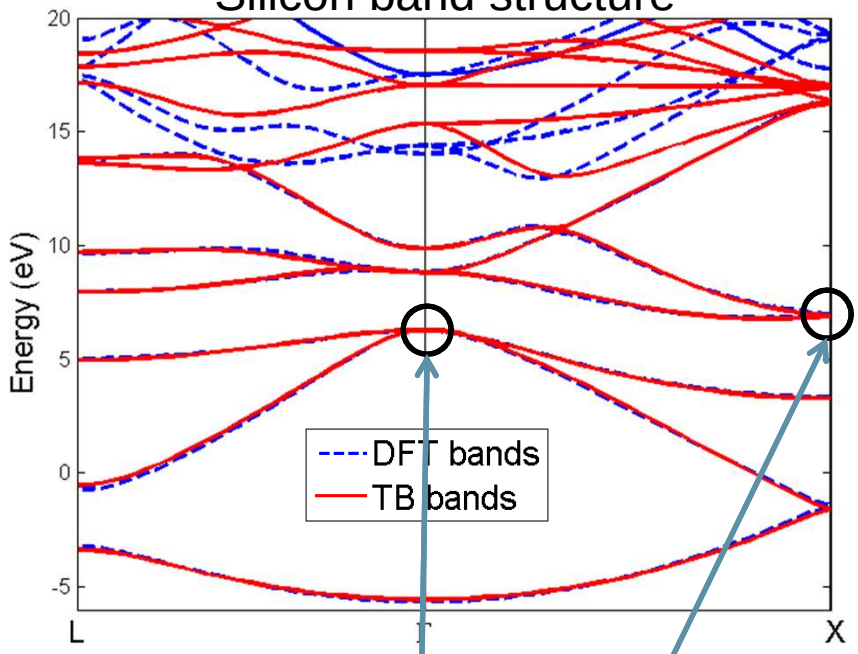
$$H_{DFT} \rightarrow H_{TB}$$

- constraint:
  - 1st NNs Interactions,
  - unity overlap matrix;
- optimize the TB basis functions to get reasonable TB parameters.
  targets: DFT bands & wavefunctions.

Results:

- Reasonable parameters and band structure is obtained by mapped TB Hamiltonian;

Silicon band structure



feature:

TB eigen functions are fitted to corresponding DFT WFs.

WFs deviation: 3% at Γ, 25% at X

Impact:

New way of getting TB parameters;
TB method now include more physics (wave functions)

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