Electronic structure calculation for broken-gap devices

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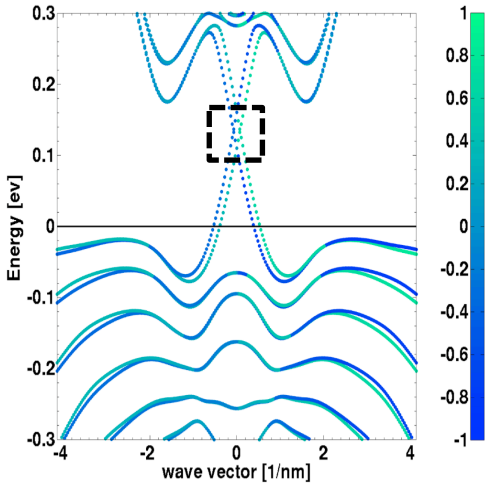
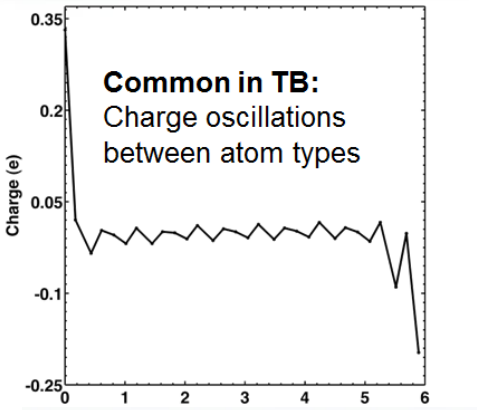
Objective

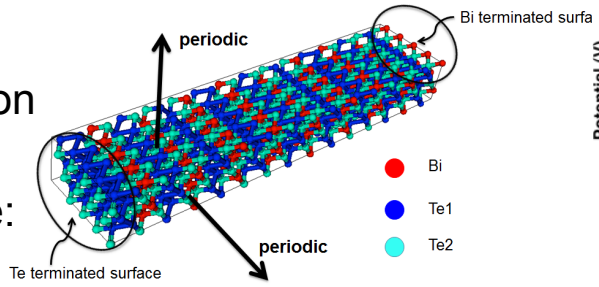
- Accurately model the eigen spectrum of broken-gap devices and topological insulators → Applicable when classical electron hole description fails

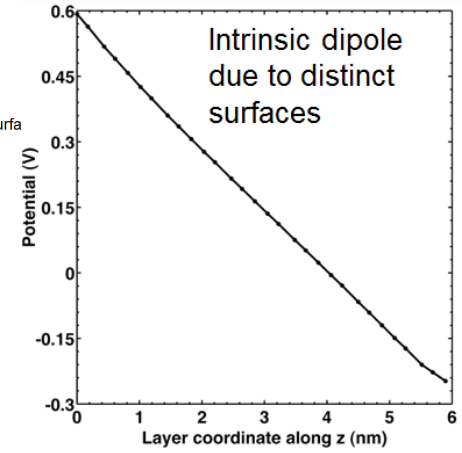
Method

- Consider all states as electronic and assume a positive charge background
- Screening of core shell electrons is neglected (ε = 1)
- Total charge density per atom = - electron density per atom + ionic charge
- To compute positive background charge: Calculate bulk density in TB
- Electron density at each atom = positive ionic charge
- Bulk parameters are transferred to heterostructures
- Self-consistently solve the Schrodinger-Poisson equation with bulk parameters









Result

- Charge self-consistent tight-binding calculation done for a Bi_2Te_3 thin-film
- Energy separation between Dirac cones gets enhanced
- Fermi velocity of Dirac states changes