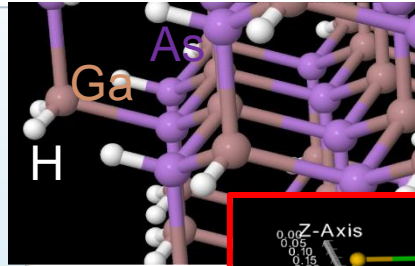


Motivation

Dangling bonds in TB-calculations result in surface states
 Surface states lie within interesting energy intervals (such as band gap)

NEMO5 - solution:

- **Implicit** inclusion of H-passivation in Hamiltonian (via self-energies)
- Efficient, no transformation required
- Allows any kind of surface



GaAs quantum well bandstructure

