Electronic Properties of Si Nanowires

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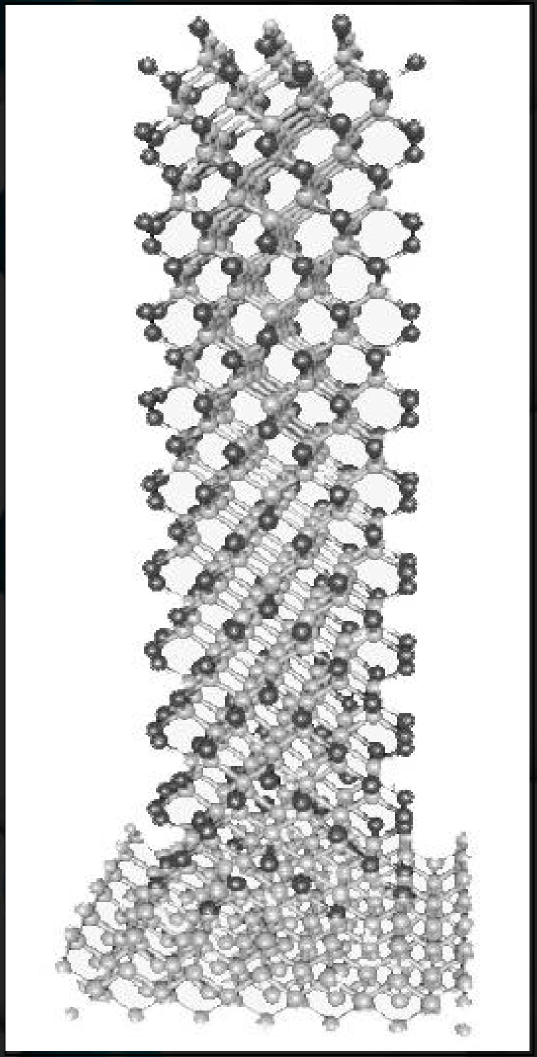
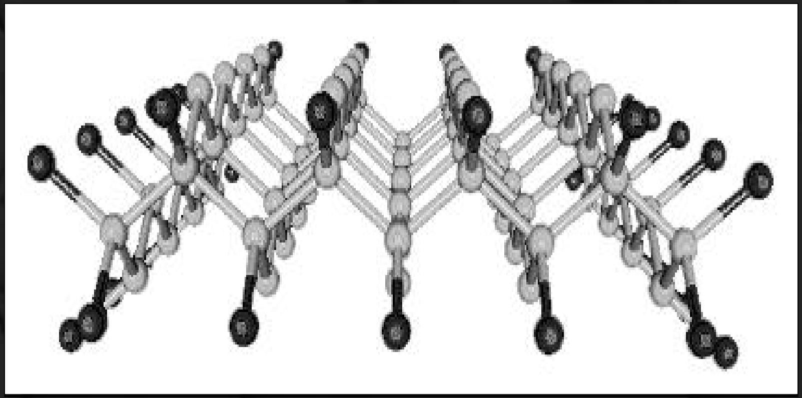
Si [100] Nanowire Structure



Si Nanowire on Si substrate



Unit Cell

H passivated

Approach

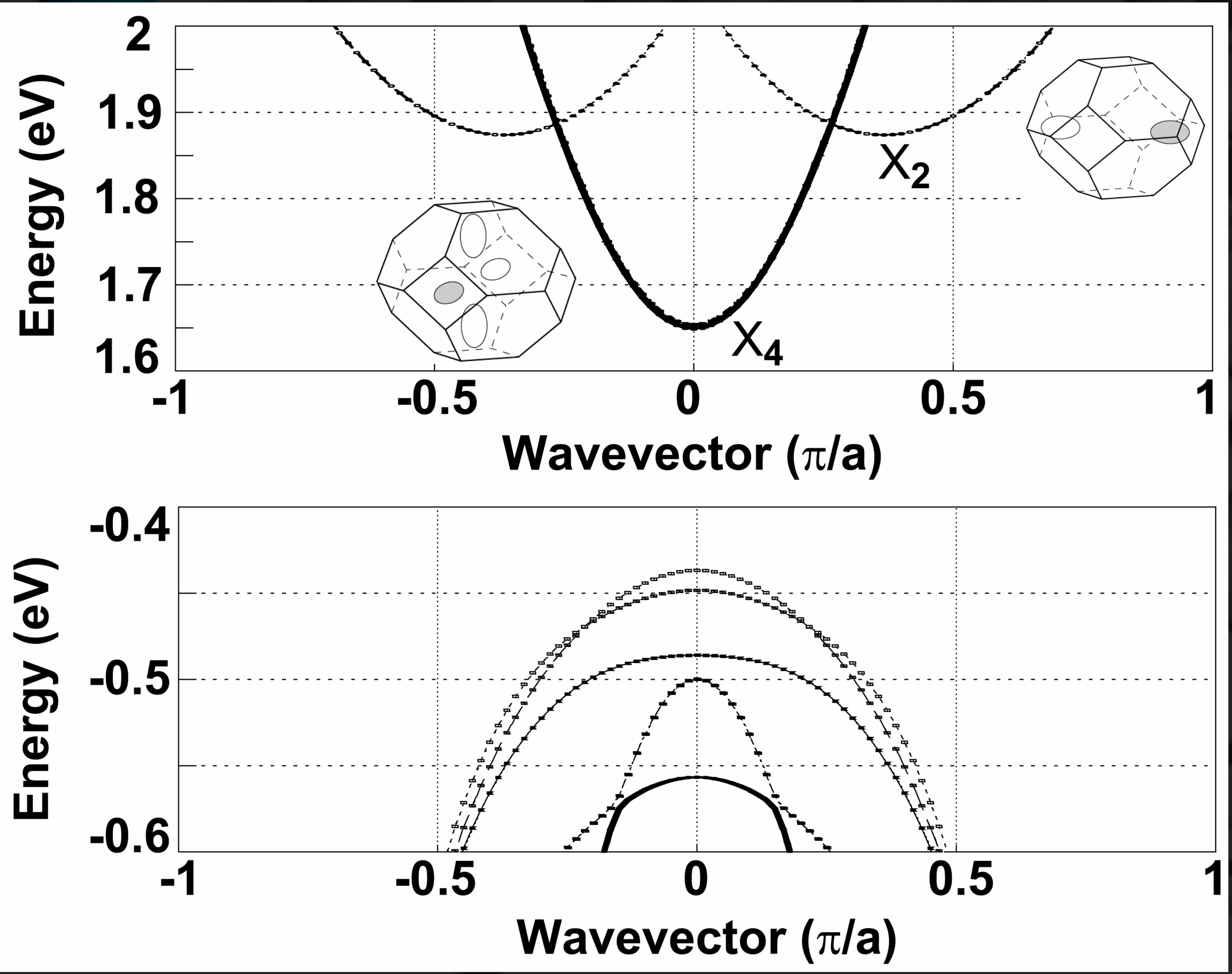
- **$sp^3s^*d^5$ empirical tight binding model**
  - **parameters optimized with genetic algorithm (Boyki** **et al., Phys. Rev. B, v. 69, 115201 (2004).**
- **3D discretized effective mass model**
- **$E - k_z$ (zeegv)**
- **Transmission vs. E**
  - **NEGF and RGF** $T = tr\{G_{1,1}[A_{1,1} - G^R_{1,1} G_{1,1} G^{R\dagger}_{1,1}]\}$

g_s^L  g_s^R

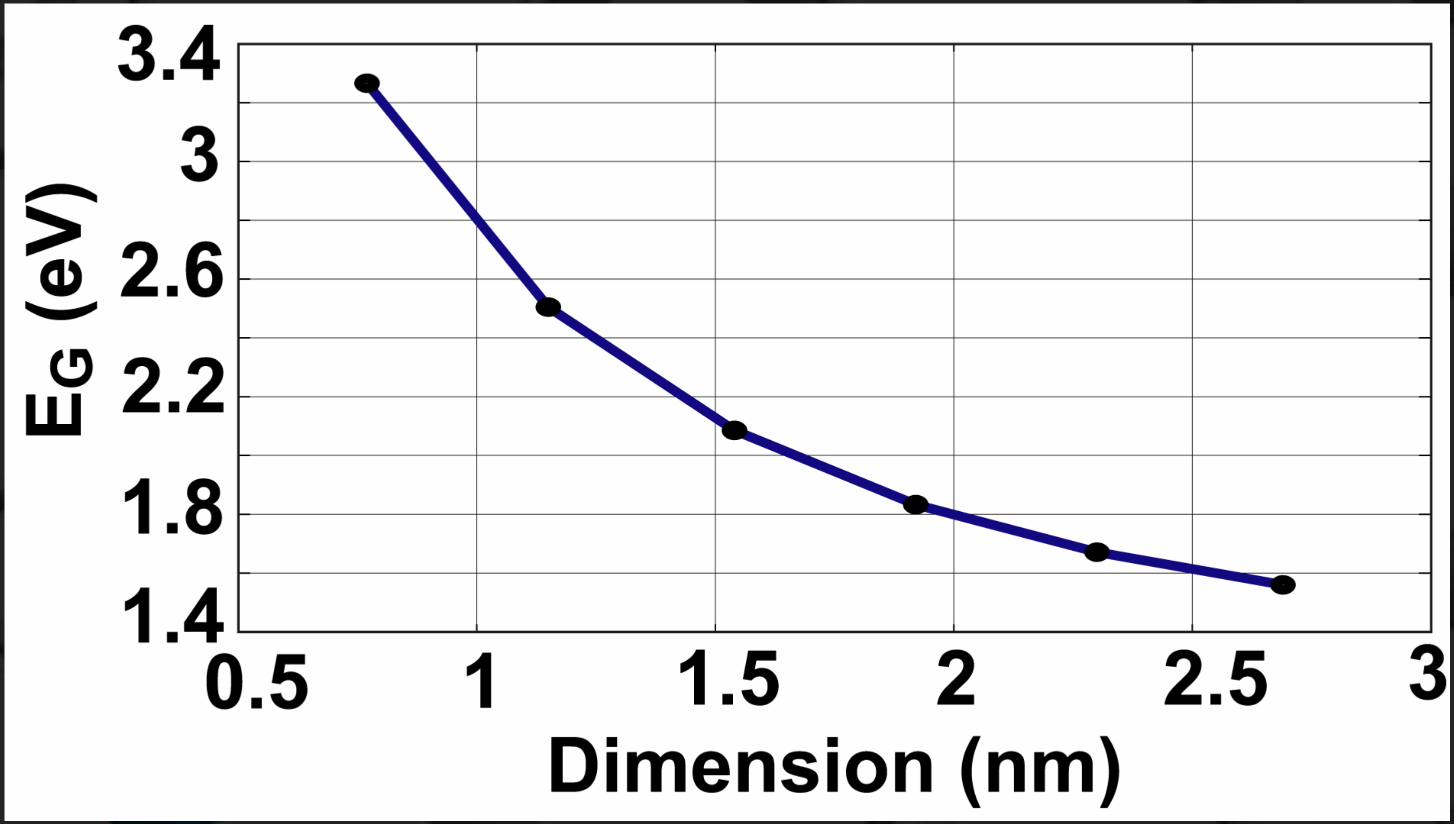
$$g^R_{i,i} = [E - D_i - t_{i,i+1}\, g^R_{i+1,i+1}\, t_{i+1,i}]^{-1}$$

$$G^R_{1,1} = [E - D_1 - t_{1,0}\, g_s^L\, t_{0,1} - t_{1,2}\, g^R_{2,2}\, t_{2,1}]^{-1}$$

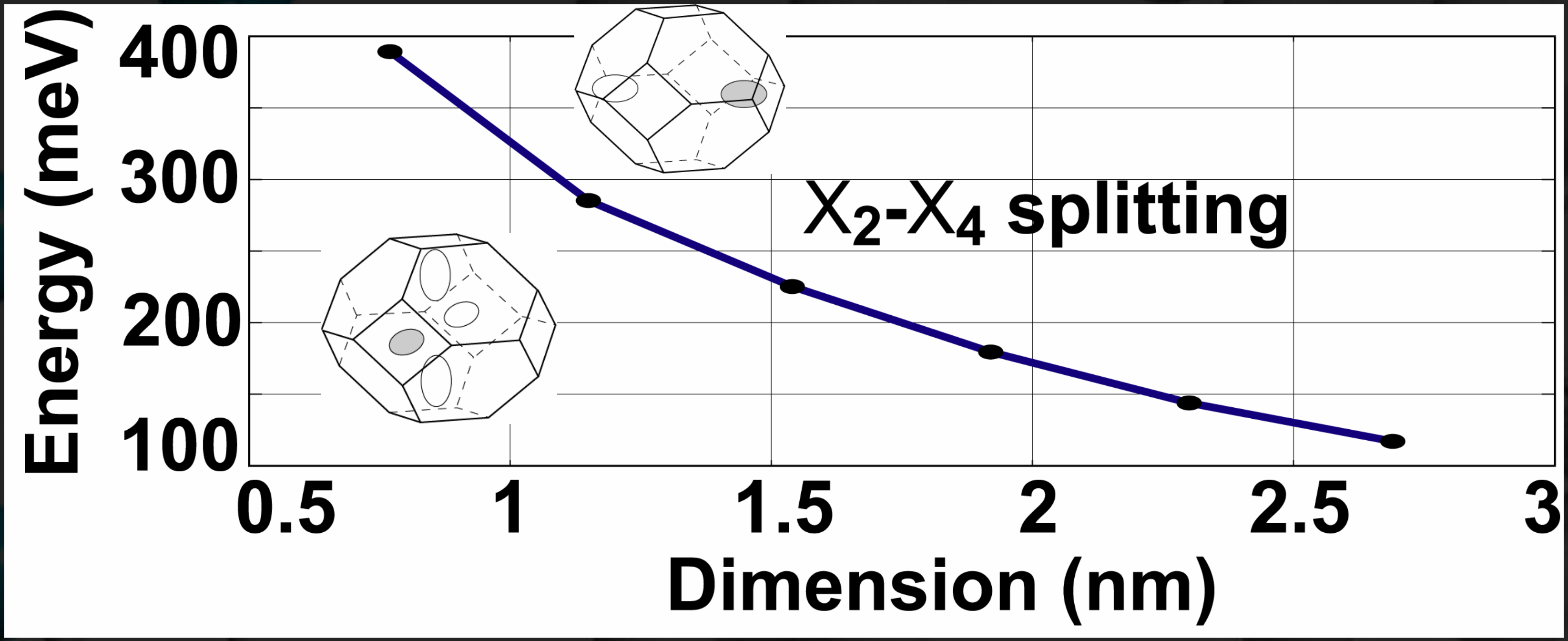
E-k_z of 1.54 nm Si Wire

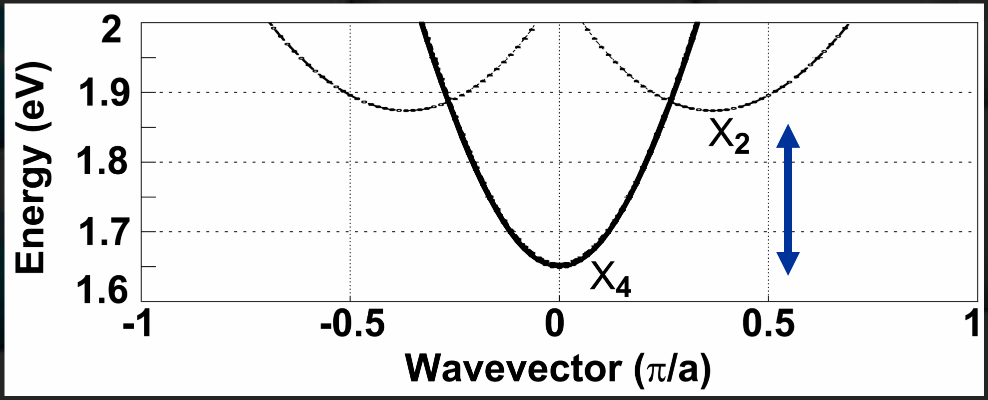


Band Gap vs. Wire Thickness

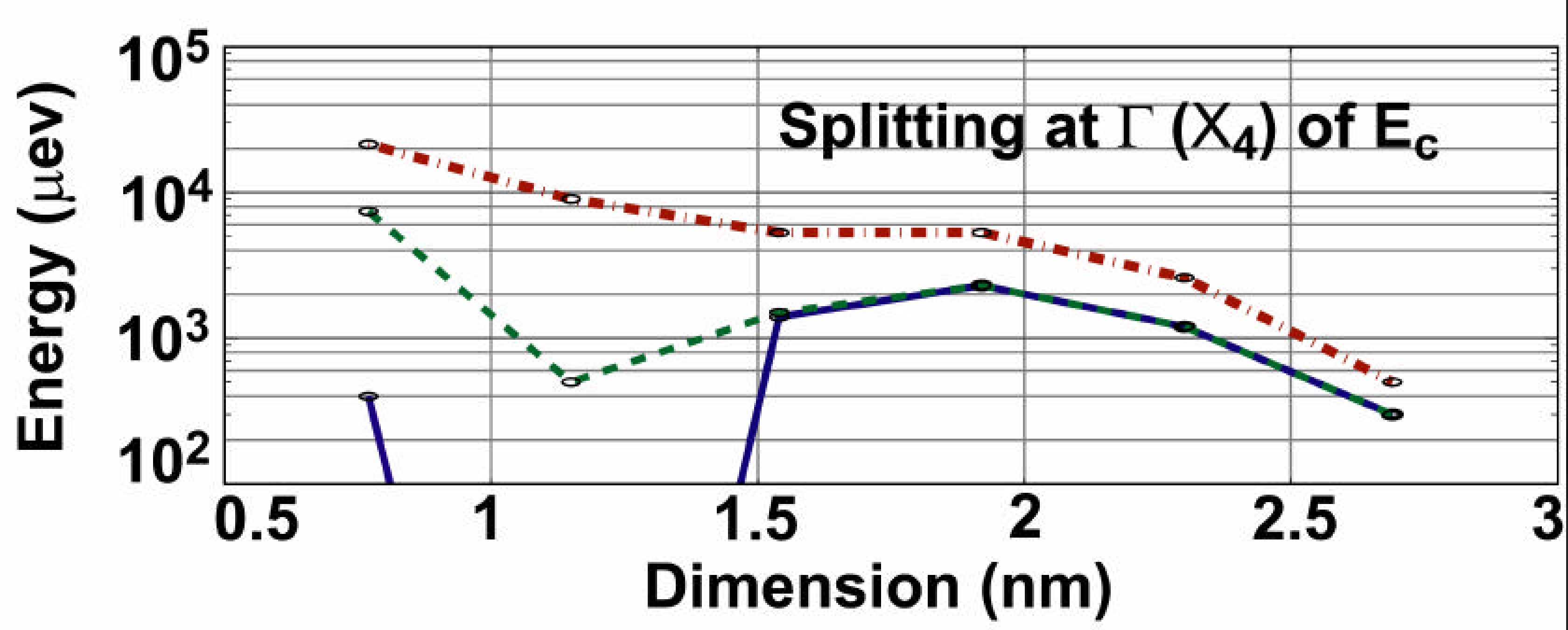


$X_2 – X_4$ Splitting

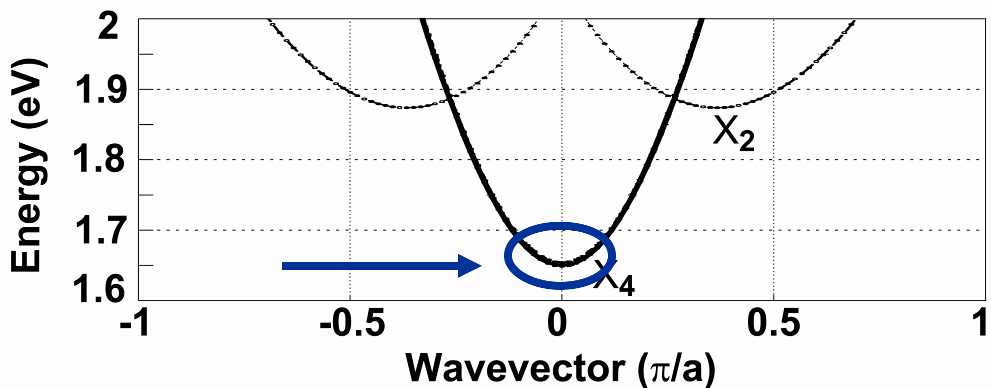




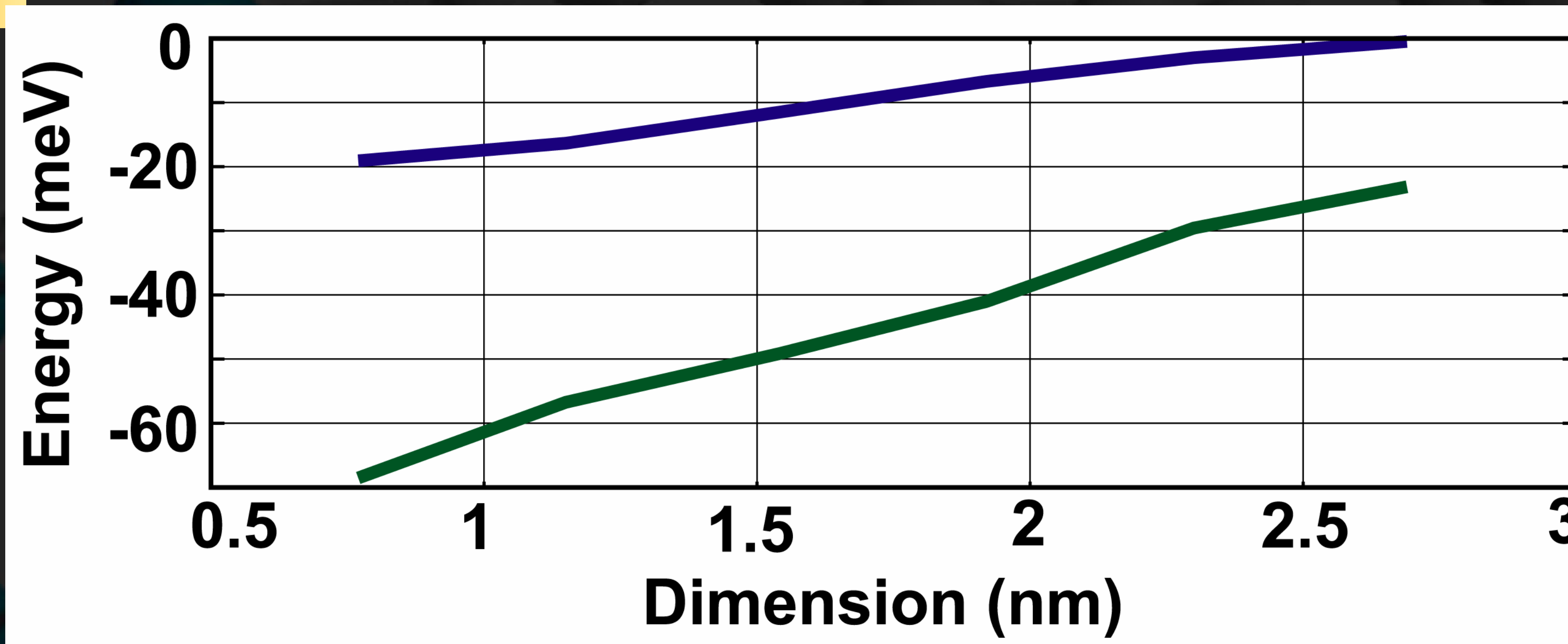
Splitting of X_4 States at Γ



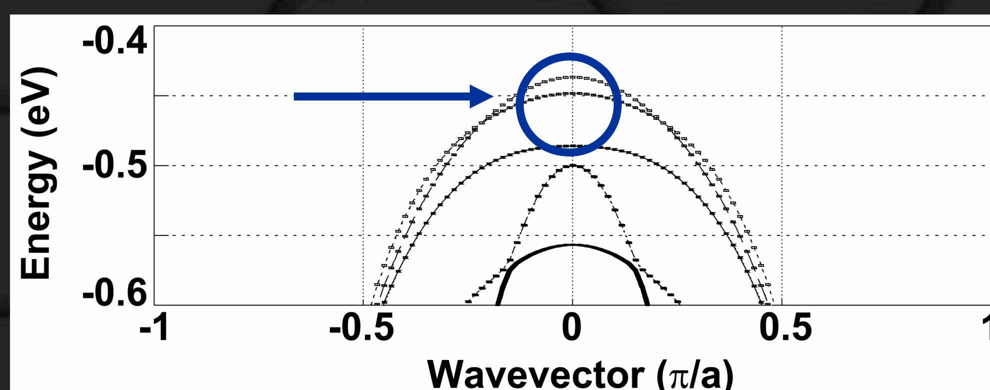
The lowest state is the reference energy E=0 at each dimension.



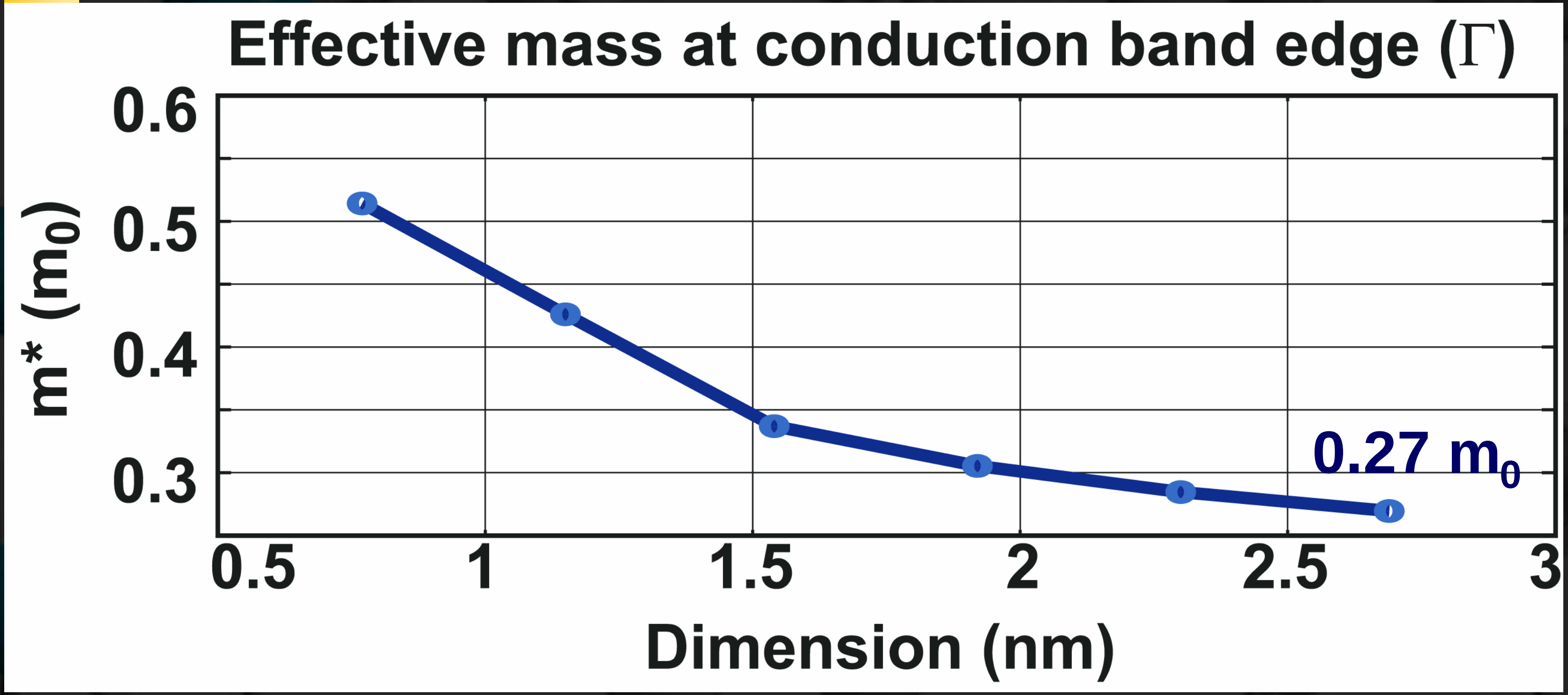
Splitting of 3 Highest Valence Bands at G



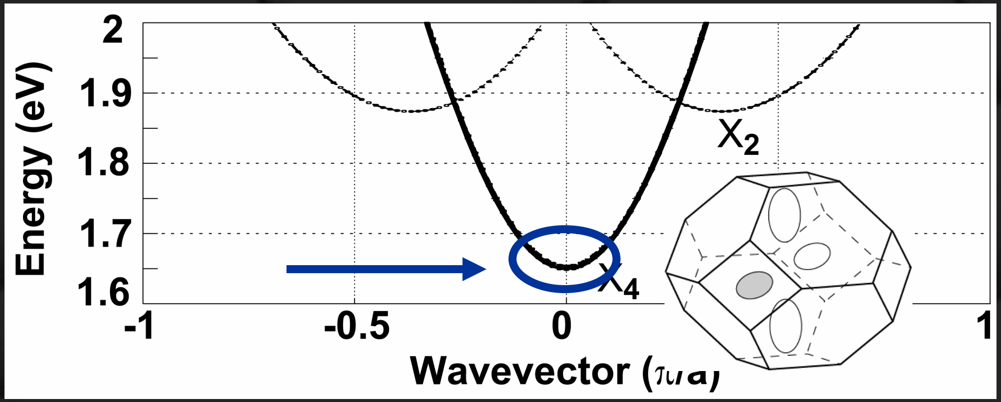
The highest state is the reference energy E=0 at each dimension.



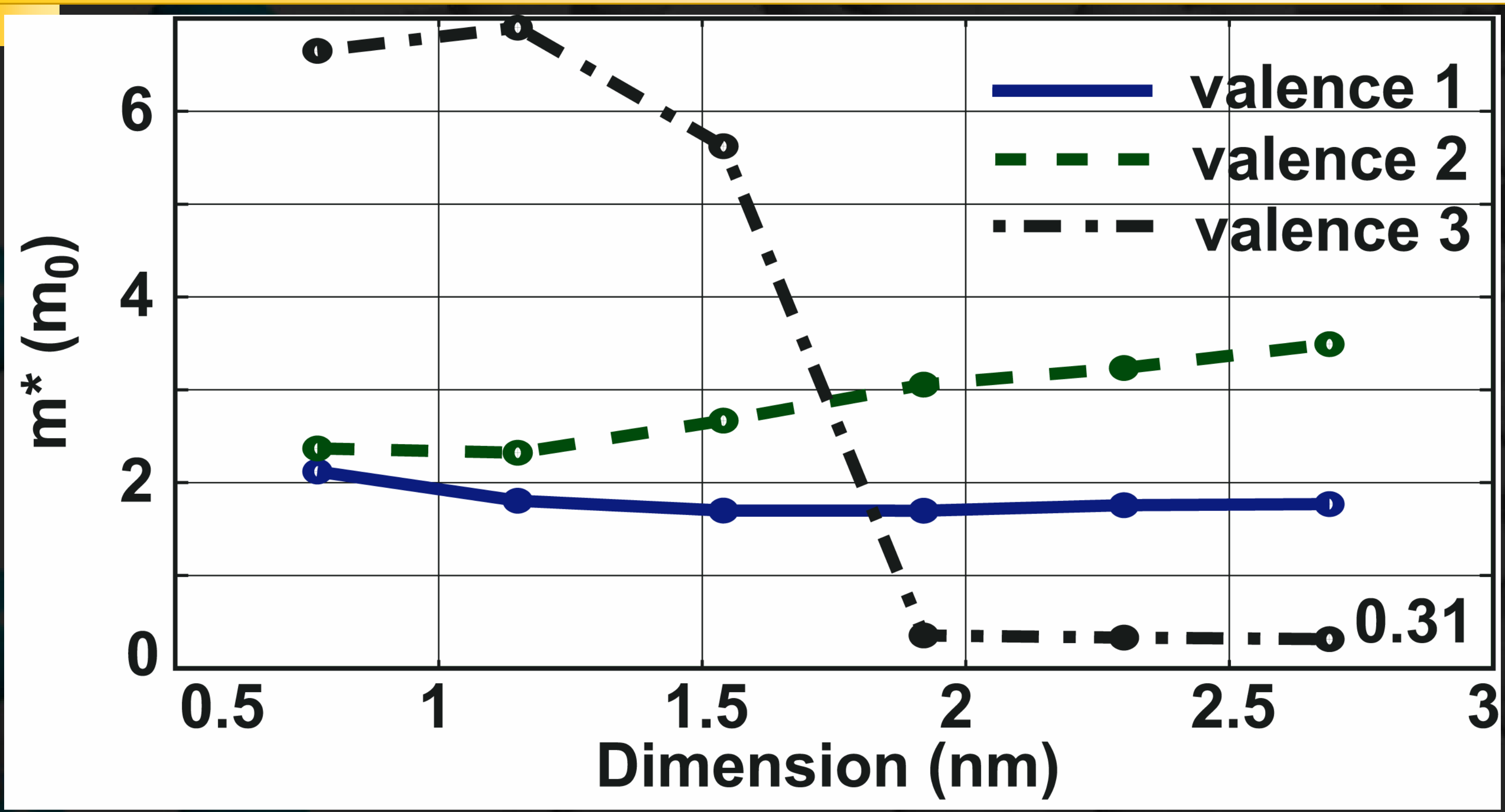
Effective Mass at Conduction Band Edge



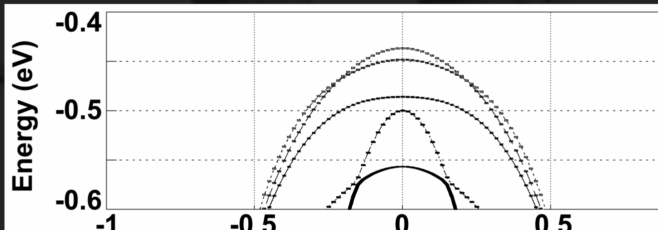
Bulk $m_t = 0.2\ m_0$



Effective Mass at Valence Band Edge



[100] bulk masses: $m_{hh} = 0.28\ m_0$, $m_{lh} = 0.21\ m_0$, and $m_{so} = 0.25\ m_0$

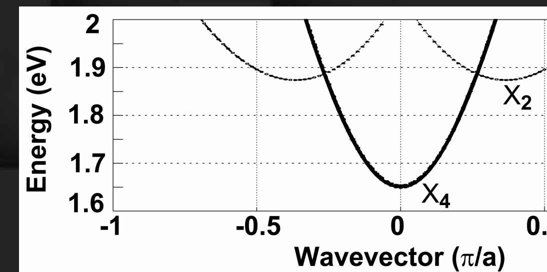


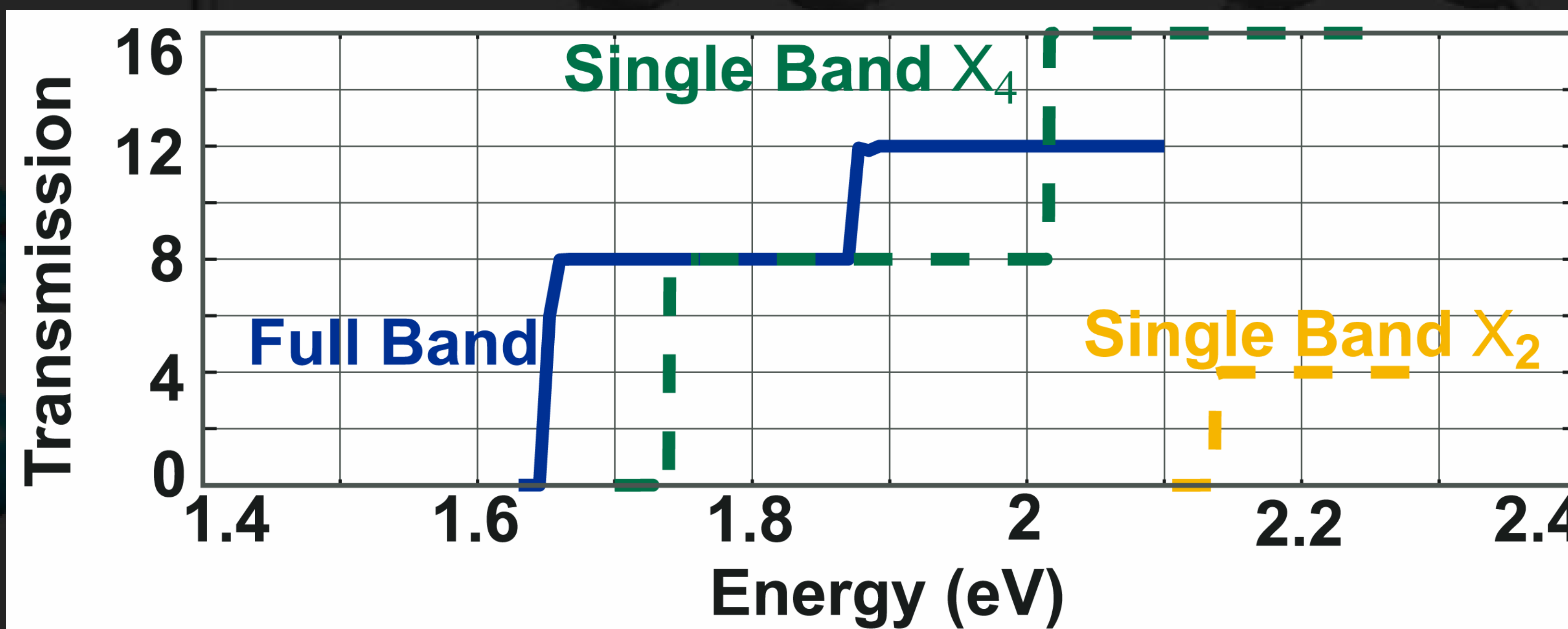
Conduction Band Transmission: Full Band and Single Band

$T = tr\{G_{1,1}[A_{1,1} - G_{1,1}G_{1,1}G_{1,1}]\}$

1.54 nm Si wire.

Band edges differ by 100 meV.

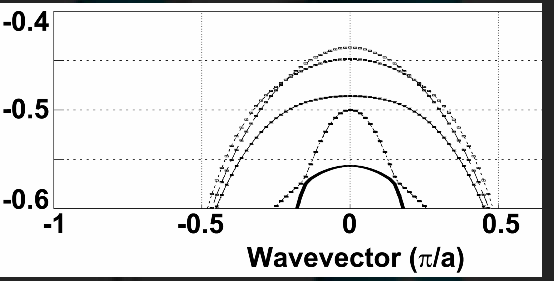


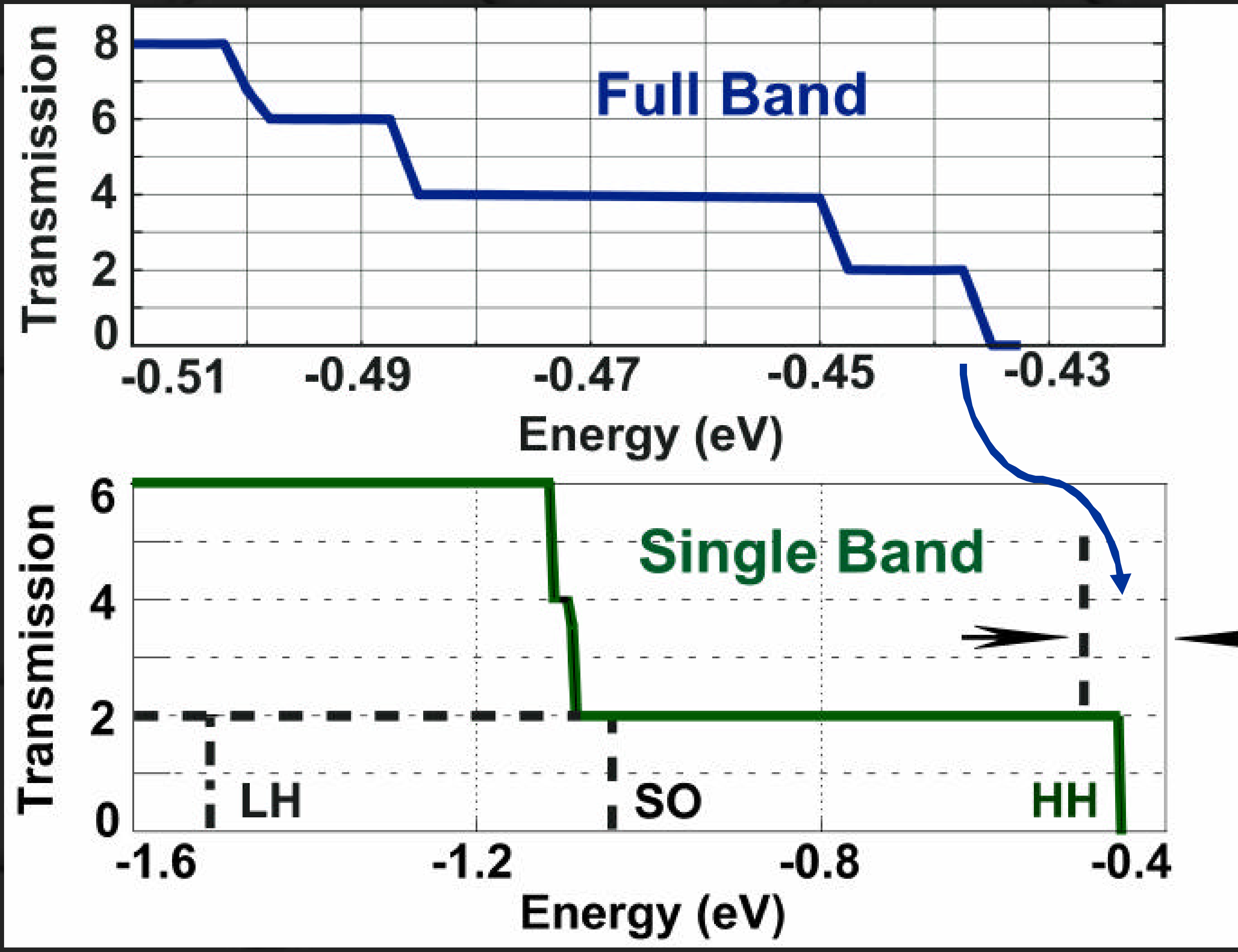


Valence Band Transmission: Full Band and Single Band

- Band edges differ by 18 meV.

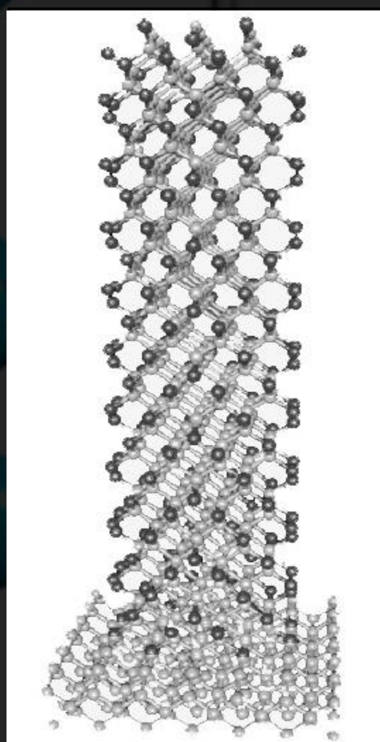
1.54 nm wire

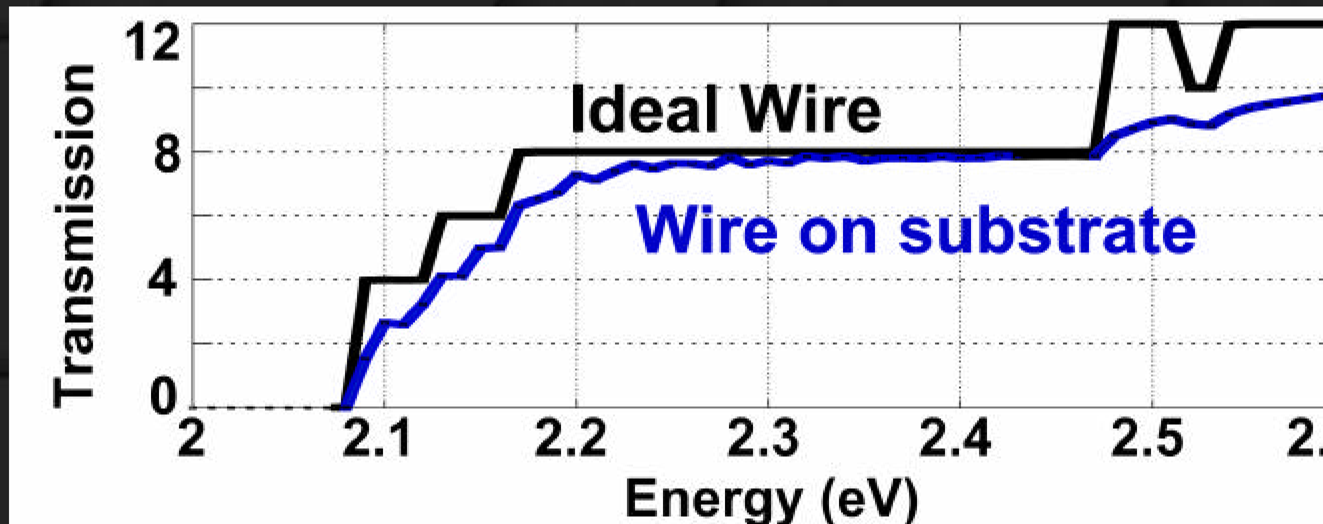


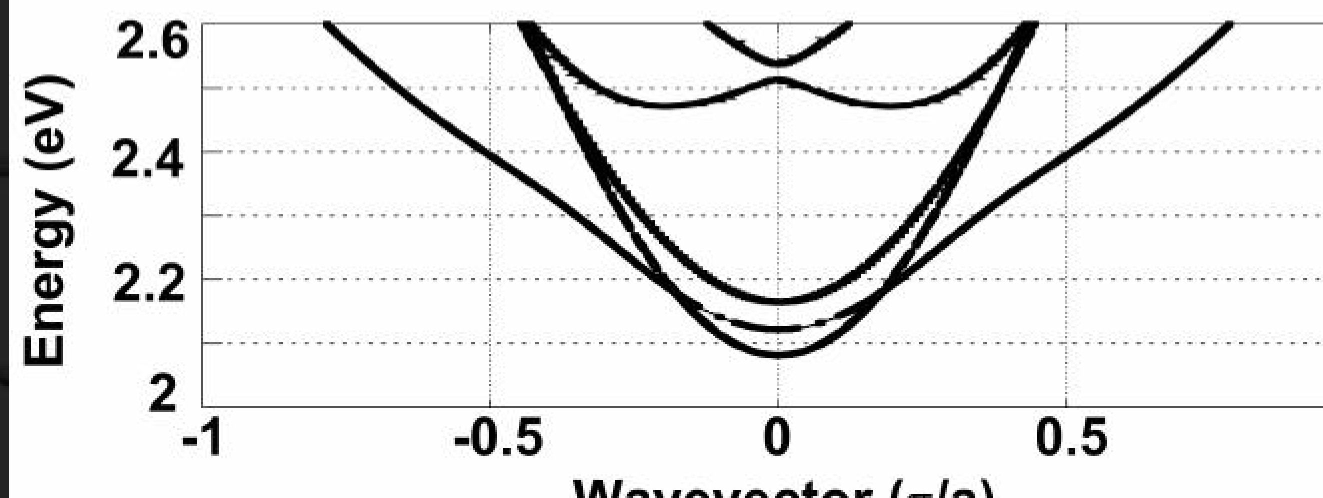


Transmission of Wire on Si Substrate

$$g_0(\mathbf{R}-\mathbf{R}';E)=\frac{1}{\Delta^2}\int\frac{d^2k}{4\pi^2}g_0(\mathbf{k}_{2d};E)\exp\left(i\mathbf{k}_{2d}\bullet(\mathbf{R}-\mathbf{R}')\right)$$







Conclusion

Brillouin zone ½ length of bulk Si along D line.

Conduction band: Valley splitting reduces m* and confinement increases m_t of bandedge (34% for 2.7nm wire).

m* of valence band edge 6x heavier than bulk and next highest band even heavier.

For wires > 1.54 nm, conduction band edge splits into 3 energies. Center energy is 2-fold degenerate evenly spaced between lowest and highest energy. Band-edge is non-degenerate.