

PHY 381C (57710) Computational Physics, Fall 2019

Project 1 (Due October 10th)

Read the paper by J. Chadi and M. Cohen, phys. stat. sol. (b) **68**, 405 (1975), and construct the tight binding Hamiltonian for crystalline Si. Calculate the band structure along the usual high symmetry directions of the *fcc* Brillouin zone: \mathbf{L} to $\mathbf{\Gamma}$ to \mathbf{X} .

Calculate and plot the band structure of Si from $\mathbf{\Gamma}$ to \mathbf{X} . Find the lowest energy state of the lowest conduction band (give the coordinates). This is your **band minimum**. Find the effective mass at this point along the $\mathbf{\Gamma X}$ direction.

Bonus question: Now calculate the band structure along a vector starting from the band minimum but pointing at 90° to the $\mathbf{\Gamma X}$ direction. Calculate the effective mass at the band minimum along this new direction.