# Problem 1

Atomic Hole doping of Graphene on SiC - Tight Binding Calculation Compared with ARPES data

A study on single layered graphene on SiC has shown that epitaxial graphene is doped by the substrate through charge transfer.[1] In the case of SiC, the Fermi level is shifted up such that the graphene is n-doped by approximately 420 meV. Angle resolved photoemission spectra (APRES) shows direct observation of the band structure of the graphene. Here we show that the band structure for graphene is not greatly altered from the tight binding theory predictions, while the Fermi level shifts dramatically back to the zero point by the addition of Bismuth.

Single Layer Tight Binding Calculations

To begin, we start with the Brillouin Zone of Graphene, shown below.
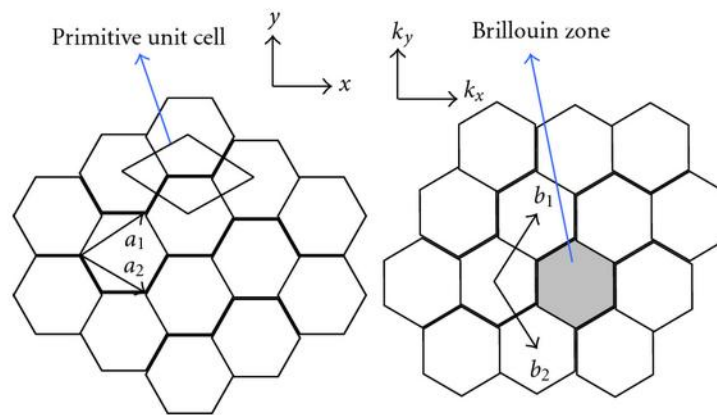
The distance between carbon atoms in real space is $a = 0.142$ nm, therefore we can see that the primitive lattice vectors are:

$$\mathbf{a}_1 = \tfrac{a}{2}(3, \sqrt{3}) \text{ and } \mathbf{a}_2 = \tfrac{a}{2}(3, -\sqrt{3})$$

Taking the Fourier Transform of real space, we find that the lattice vectors for the reicprocal space are:

$$\mathbf{b}_1 = \tfrac{2\pi}{3a}(1, \sqrt{3}) \text{ and } \mathbf{b}_2 = \tfrac{2\pi}{3a}(1, -\sqrt{3})$$

Starting with the assumption of a linear combination of atomic orbitals (LCAO), we find the ground state of an single electron $\psi_{\mathbf{k}}(\mathbf{r})$ moving through a potential of an isolated atom $U(\mathbf{r})$. We then notice that if the electrons are in the s state and therefore have little affect on each other (i.e. the wavefunctions are linearly independent), then we can construct an approximate wavefunction for a single electron within the whole crystal lattice (rather than a single atom):

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \sum_{j} C_{j\mathbf{k}} \psi_{\mathbf{k}}(\mathbf{r}) \tag{1}$$

Where j is each lattice point within the crystal. We remember now that the solution to the Schödinger Equation for a periodic potential is of the Bloch function form (Kittel Equation 7.7):

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \tag{2}$$

Where $|\Psi\rangle$ is the

References

[1] GIERZ, I., RIEDL, C., STARKE, U., AST, C. R., AND KERN, K. Atomic hole doping of graphene. *Nano letters 8*, 12 (2008), 4603–4607.