First-Principles Screening of Dopants for High-Conductivity Graphene/Copper Interfaces- Supplementary Material

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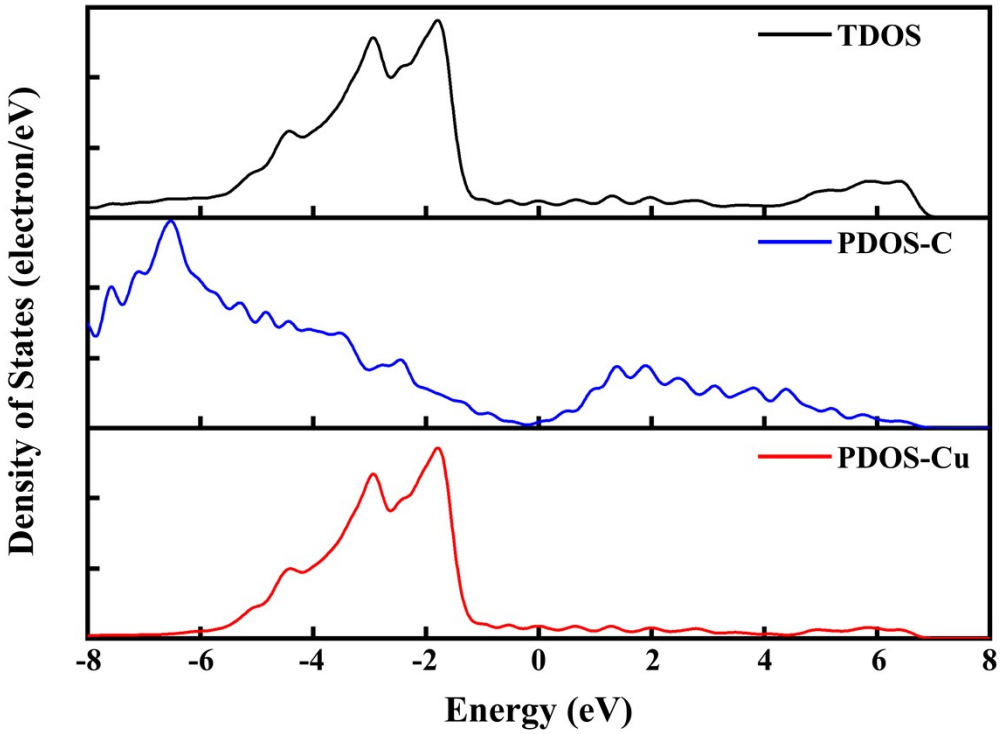

Fig. S1. The DOS of the Gr/Cu interface.

derivation of equation

$$E_F = \hbar v_F \sqrt{\pi n} \tag{eq.1}$$

For two-dimensional material like suspended Gr, it has a zero bandgap and linear dispersion relation

$$E(k) = \hbar v_F k \tag{eq.2}$$

The electrons are all in a plane of radius k in k-space. The degeneracy of Gr is 4, which from spin degeneracy and valley degeneracy. Thus the number of states is

$$\begin{aligned} N(E) &= 4 \cdot \frac{S}{(2\pi)^2} \cdot \pi k^2 \\ &= \frac{2SE^2}{\pi \hbar^2 v_F^{\,2}} \end{aligned} \tag{eq.3}$$

The number of states per unit energy interval is

$$D(E) = \frac{dN(E)}{dE} = \frac{d\left(\frac{SE^2}{2\pi\hbar^2 v_F^{\,2}}\right)}{dE} = \frac{2SE}{\pi \hbar^2 v_F^{\,2}} \tag{eq.4}$$

The number of states per unit area is

$$g(E) = \frac{2E}{\pi \hbar^2 v_F^{\,2}} \tag{eq.5}$$

The electron distribution near the Fermi level follows the Fermi-Dirac statistics

$$f(E) = \frac{1}{e^{E - E_F / K_B T} + 1} \tag{eq.6}$$

Simplifying this equation, when there are electrons, $f(E)$=1; when there are unoccupied, $f(E)$=0.

The carrier concentration can be calculated by

$$n = \int_0^{E_F} g(E) f(E) dE = \int_0^{E_F} \frac{2E}{\pi \hbar^2 v_F^{\,2}} dE = \frac{E_F^2}{\pi \hbar^2 v_F^{\,2}} \tag{eq.7}$$

Which can be written as

$$E_F = \hbar v_F \sqrt{\pi n} \tag{eq.1}$$

$$n = \frac{m^*}{\pi\hbar^2}\Delta E \quad \text{(eq.8)}$$

When doping in Gr of Gr/Cu composite induced bandgap opening, the linearity may be disrupted. The same derivation is used to derive the equation for the carrier concentration under the parabolic band.

The relationship between energy ($E(k)$) and wave vector (k) is

$$E(k) = \frac{\hbar^2 k^2}{2m^*} \quad \text{(eq.9)}$$

The number of states is

$$\begin{aligned} N(E) &= 2 \cdot \frac{S}{(2\pi)^2} \cdot \pi k^2 \\ &= 2 \cdot \frac{S}{(2\pi)^2} \cdot \pi \cdot \frac{2m^* E}{\hbar^2} \\ &= \frac{Sm^* E}{\pi\hbar^2} \end{aligned} \quad \text{(eq.10)}$$

The number of states per unit energy interval is

$$D(E) = \frac{dN(E)}{dE} = \frac{d(\frac{Sm^* E}{\pi\hbar^2})}{dE} = \frac{Sm^*}{\pi\hbar^2} \quad \text{(eq.11)}$$

The number of states per unit area is

$$g(E) = \frac{m^*}{\pi\hbar^2} \quad \text{(eq.12)}$$

The carrier concentration can be calculated by

$$n = \int_0^{E_F} g(E)f(E)dE = \int_0^{E_F} \frac{m^*}{\pi\hbar^2}dE = \frac{m^*}{\pi\hbar^2}E_F \quad \text{(eq.13)}$$

Which can be written as

$$n = \frac{m^*}{\pi\hbar^2}\Delta E \quad \text{(eq.8)}$$