Supporting information for: Porous Graphene-Fullerene Nanocomposites: A New Composite for Solar Cell and Optoelectronic Applications

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1 Supporting Information

1. Explanation of different optical parameters.

2. The total density of states of a representative isolated PG and the projected density of states of PG in its corresponding PG-C_{60} composite.

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The complex dielectric function $\varepsilon = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ is used to calculate the optical properties of a system, where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ represent the real and imaginary part of the dielectric function, respectively. The imaginary part which mainly originates from the interband transition, can be obtained from the Fermi's golden rule as

$$\varepsilon_2(\omega) = \frac{4\pi^2}{\Omega\omega^2} \sum_{i\in VB, j\in CB} \sum_k W_k |\rho_{ij}^a|^2 \delta(\varepsilon_{kj} - \varepsilon_{ki} - \omega) \tag{1}$$

where Ω is the unit cell volume and ω represents the frequency of the electromagnetic radiation, in terms of unit of energy. ρ_{ij} is the dipole transition matrix element that can be expressed as $< k_j|\hat{p}_\alpha|k_i >$ and can be obtained from self-consistent band structure. The real part of the dielectric function can be obtained by Kramers-Kronig transformation as

$$\varepsilon_1(\omega) = 1 + \frac{4}{\pi} P \int_0^\infty d\omega' \frac{\omega' \varepsilon_1(\omega')}{\omega'^2 - \omega^2} \tag{2}$$

The imaginary and real part of dielectric function can be calculated and using these set of data, other optical properties such as absorption coefficient $\alpha(\omega)$, optical conductivity $\sigma(\omega)$, reflectivity R(ω)and refractive index $\eta(\omega)$ can be obtained. The absorption coefficient is the fraction of energy lost by the wave when the electromagnetic wave passes through a unit thickness of the materials.

$$\alpha(\omega) = \sqrt{2}\omega \left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega) \right]^{\frac{1}{2}} \tag{3}$$

$$\sigma(\omega) = -i\frac{\omega}{4\pi} |\varepsilon(\omega) - 1| \tag{4}$$

$$R(\omega) = \left[\frac{\sqrt{\varepsilon_1(\omega) + i\varepsilon_2(\omega)} - 1}{\sqrt{\varepsilon_1(\omega) + i\varepsilon_2(\omega)} + 1} \right]^2 \tag{5}$$

$$\eta(\omega) = \frac{\left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} + \varepsilon_1(\omega) \right]^2}{\sqrt{2}} \tag{6}$$

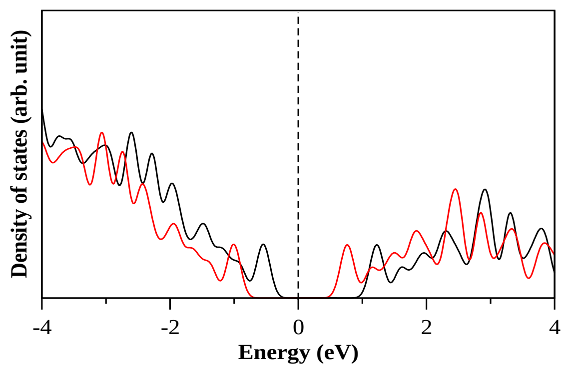

Figure S1: **The total density of states of a representative isolated PG (black line) and the projected density of states (red line) of PG in PG-C_{60} composite.**