Supporting Information

Improving Dispersion and Barrier Properties of Polyketone/Graphene Nanoplatelet Composites via Noncovalent Functionalization Using Aminopyrene

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Table S1. Characterizations for non-covalently functionalized GNP with Py and APy: XPS measurement, Raman spectra, thickness information by AFM.

Sample	**XPS** (atom %)				**Raman,** (I_D/I_G ratio)	**AFM,** (Thickness, nm)
	C_{1s}	O_{1s}	N_{1s}	sp^2 C		
GNP	96.7	3.2	0.1	57.6	0.03	25.01 ± 2.3
GNP/Py	95.1	4.6	0.3	64.3	0.10	7.03 ± 0.8
GNP/APy	93.6	4.4	2.0	60.0	0.07	7.21 ± 1.2

AFM analysis

The average thickness and its standard deviation of particles is calculated with 10 scans of tapping mode AFM measurements.

The fact that GNP/Py had a thinner thickness than that of GNP/APy can be explained as follows. When the pyrene moieties adsorb graphene through π-π* interaction, the affinity of the non-covalent interaction between the pyrene moieties and GNP can change due to variation of the electron density on the basal plane of pyrene. When polar functional groups such as carboxylic acid and amine functional groups are attached to pyrene (so called pyrenecarboxylic acid and aminopyrene), polarization occurs. When the electronegativity of the functional group is low, or when the electron-withdrawing group is weak, the electron density on the basal plane of pyrene increases and decreases its affinity, respectively, to the graphene basal plane. Therefore, the amine functional group of APy has a lower affinity to graphene, resulting in a lowered effectiveness of the exfoliation process of graphene.[1]

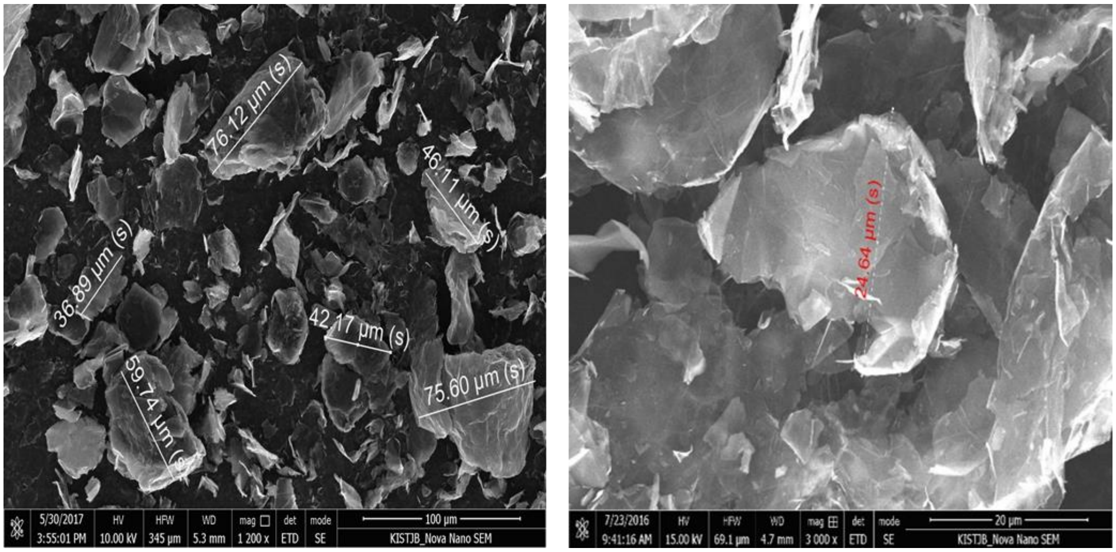

Figure S1. FE-SEM image of GNP as received (left) and GNP after sonication (right).

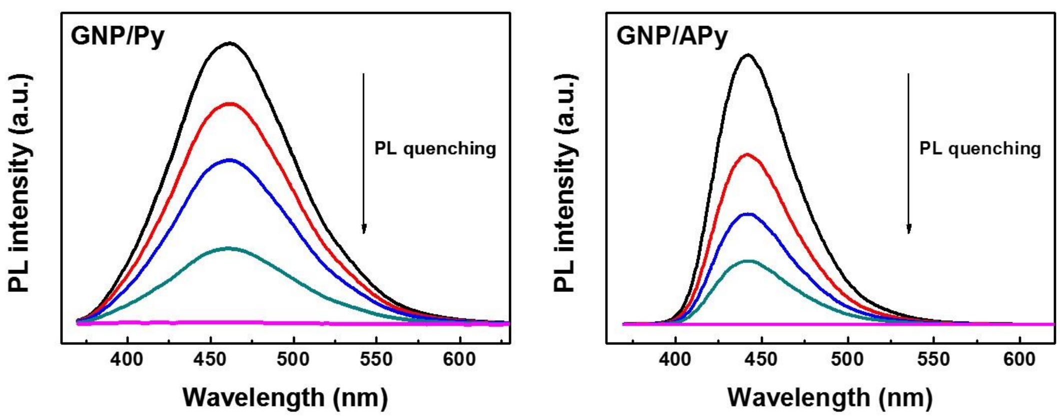

Figure S2. Fluorescence spectra of GNP/Py and GNP/APy in water.

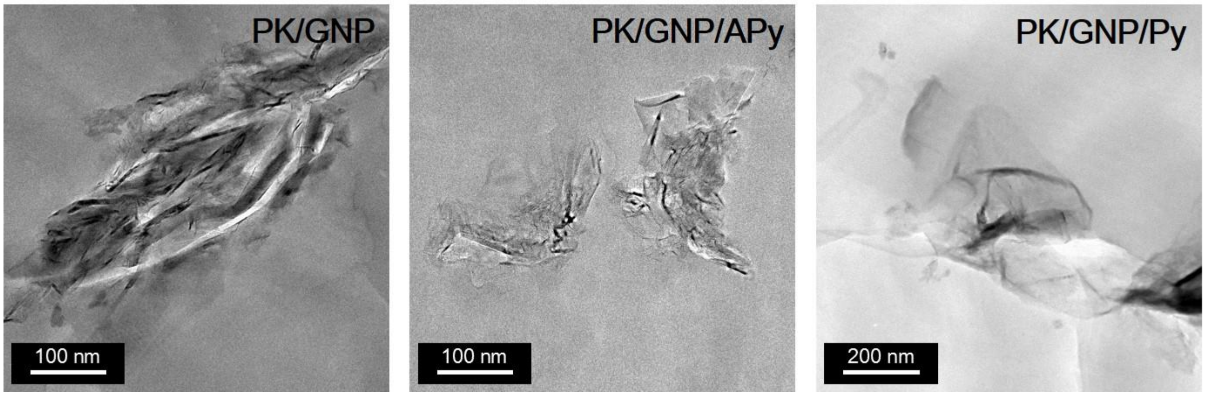

Figure S3. TEM image of GNP and f-GNP in PK matrix.

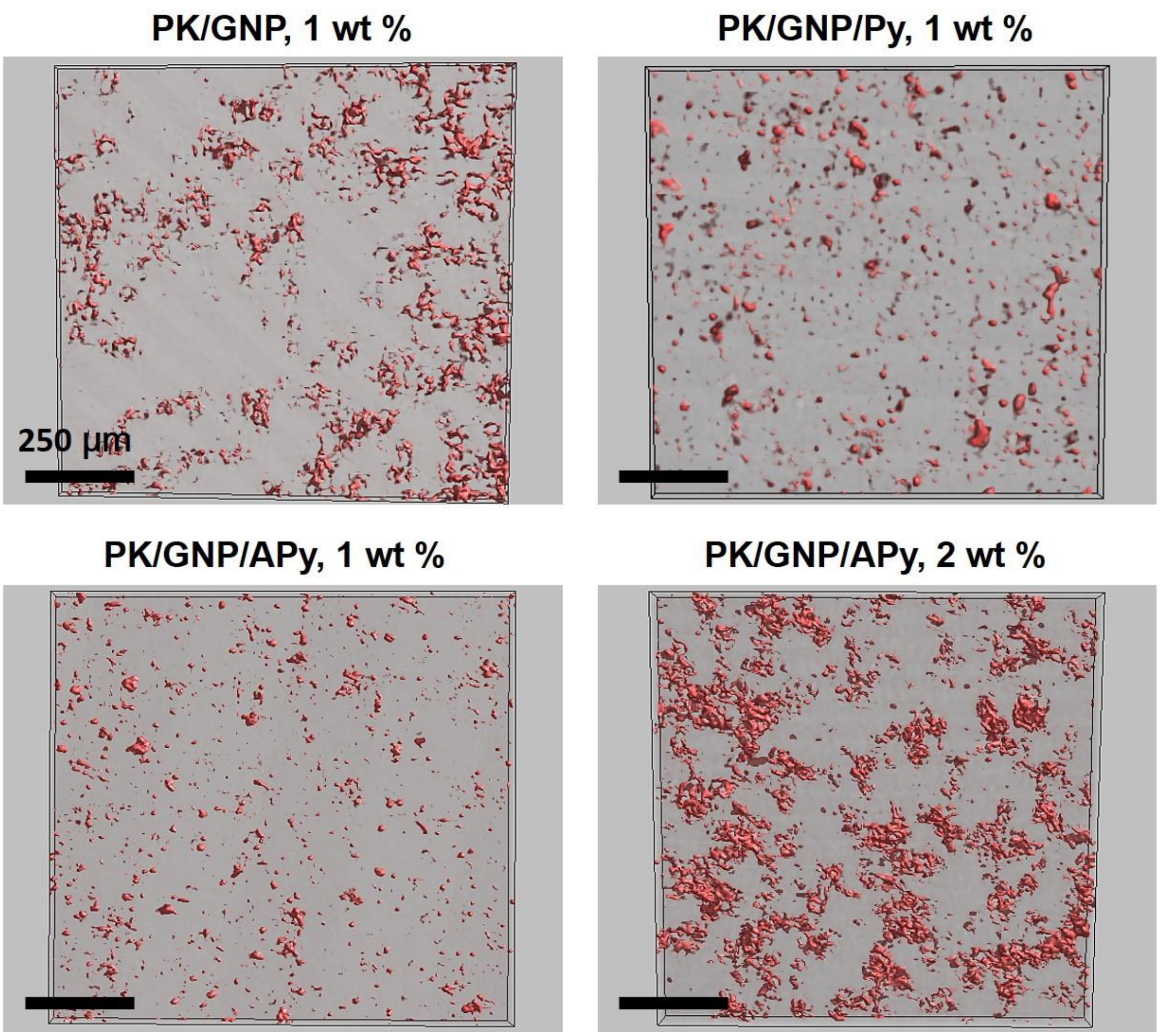

Figure S4. 3D micro CT images of PK nanocomposite films (scale bars, 250 μm).

Table S2. Properties of PK/GNP composites: Glass transition temperature measurement, Mechanical properties, Barrier properties.

Sample Code	**Filler Content** (wt %)	**Glass Transition Temperature,** (°C)	**Young's Modulus,** (MPa)	**Tensile Strength,** (MPa)	**Elongation at Break,** (%)	**WVTR,** (g/m^2-day)
PK		26.1	1583.7	56.9	20.2	28
PK/GNP	0.5	34.2	1703.2	59.2	11.8	5.9
	1		1968.6	58.0	11.0	4.2
	2		2150.1	56.3	8.1	3.5
PK/GNP/Py	0.5	36.0	1802.3	60.1	12.3	4.1
	1		2013.4	59.2	11.0	2.6
	2		2201.2	56.0	8.5	2.5
PK/GNP/APy	0.5	41.5	1873.1	64.0	17.0	3.3
	1		2150.1	67.3	13.6	2.3
	2		2293.3	59.9	10.3	2.0

Equations

Equation S1

$$\mathrm{E}_{random} = \mathrm{E}_m \left[\frac{3}{8}\left(\frac{1+\xi\eta_L\nu_f}{1-\eta_L\nu_f}\right) + \frac{5}{8}\left(\frac{1+2\eta_T\nu_f}{1-\eta_T\nu_f}\right)\right] \quad \text{(S1)}$$

Where

Equation S1-1, S1-2, and S1-3

$$\eta_L = \frac{(\mathrm{E}_f/E_m)-1}{(E_f/E_m)+\xi} \quad \text{(S1-1)}$$

$$\eta_T = \frac{(\mathrm{E}_f/E_m)-1}{(E_f/E_m)+2} \quad \text{(S1-2)}$$

$$\xi = (\frac{2}{3}\alpha_f) \quad \text{(S1-3)}$$

where E_{random} is the predicted elastic modulus of the composite filled with randomly oriented fillers, and E_m and E_f are the elastic modulus of matrix and filler, respectively. ν is filler volume fraction, α_f is the aspect ratio of the filler.

Equation S2

$$\mathrm{P}_{comp} = \mathrm{P}_m \left(\frac{1-\phi_f}{1+\alpha_f\phi_f}\right) \quad \text{(S2)}$$

where P_{comp} and P_m are the permeability of the composite and the matrix, respectively. ϕ_f refers to the filler volume fraction and α_f is the aspect ratio of the filler.

(1) Parviz, D.; Das, S.; Ahmed, H. S. T.; Irin, F.; Bhattacharia, S.; Green, M. J., Dispersions of Non-Covalently Functionalized Graphene with Minimal Stabilizer. *ACS Nano* **2012,** *6*, 8857-8867.