Electronic Supplementary Information

Table S1. Energies of the β-CD molecule, graphene, and β-CD/graphene composites (in kcal mol^{-1}).

Configurations	Valence energy	Non-bond energy			Total enthalpy
		Hydrogen bond	**van der Waals**	Electrostatic	
β-CD	108.2890	0.000	**102.07800**	0.000	210.36706
p-GE	3737.558	0.000	**10026.131**	0.000	13763.689
d-GE	3714.623	0.000	**10174.298**	0.000	13888.921
p-GE-CD head	3850.307	0.000	**10068.935**	0.000	13919.242
p-GE-CD tail	3851.073	0.000	**10086.888**	0.000	13937.962
d-GE-CD head	3833.963	0.000	**10213.000**	0.000	14045.741
d-GE-CD tail	3829.926	0.000	**10219.600**	0.000	14049.524
Binding energy					
p-GE-CD head	4.460	0.000	**-59.274**	0.000	-54.8142
p-GE-CD tail	5.226	0.000	**-41.321**	0.000	-36.0942
d-GE-CD head	11.051	0.000	**-64.599**	0.000	-53.5471
d-GE-CD tail	7.014	0.000	**-56.776**	0.000	-49.7641

$E_{Binding\ energy} = E_{\beta\text{-CD/graphene}} - (E_{graphene} + E_{\beta\text{-CD}})$.

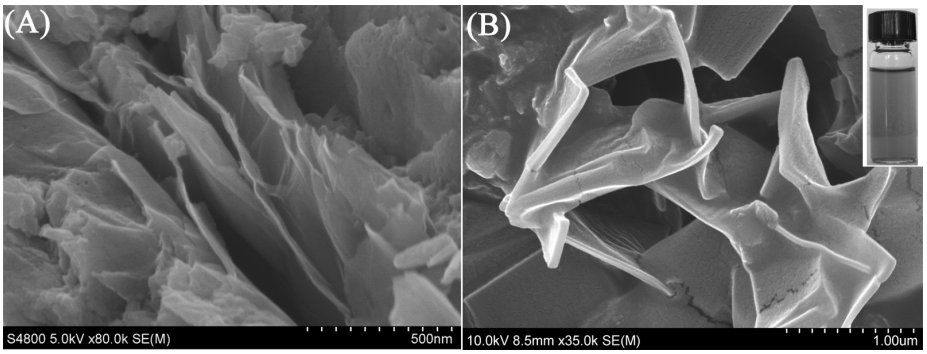

Figure S1. The SEM images of reduced graphene oxide before (A) and after (B) noncovalently functionalized of β-cyclodextrins. The inset of B is the photo of its aqueous dispersion. (c = 0.1 mg mL^{-1})

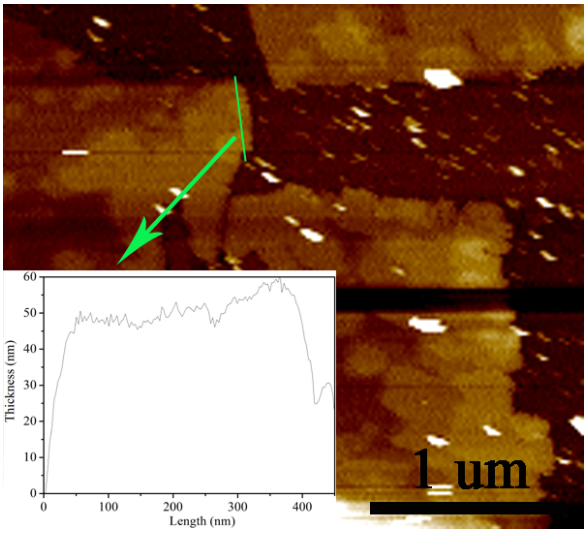

Figure S2. AFM image and the corresponding thickness distribution (inset).

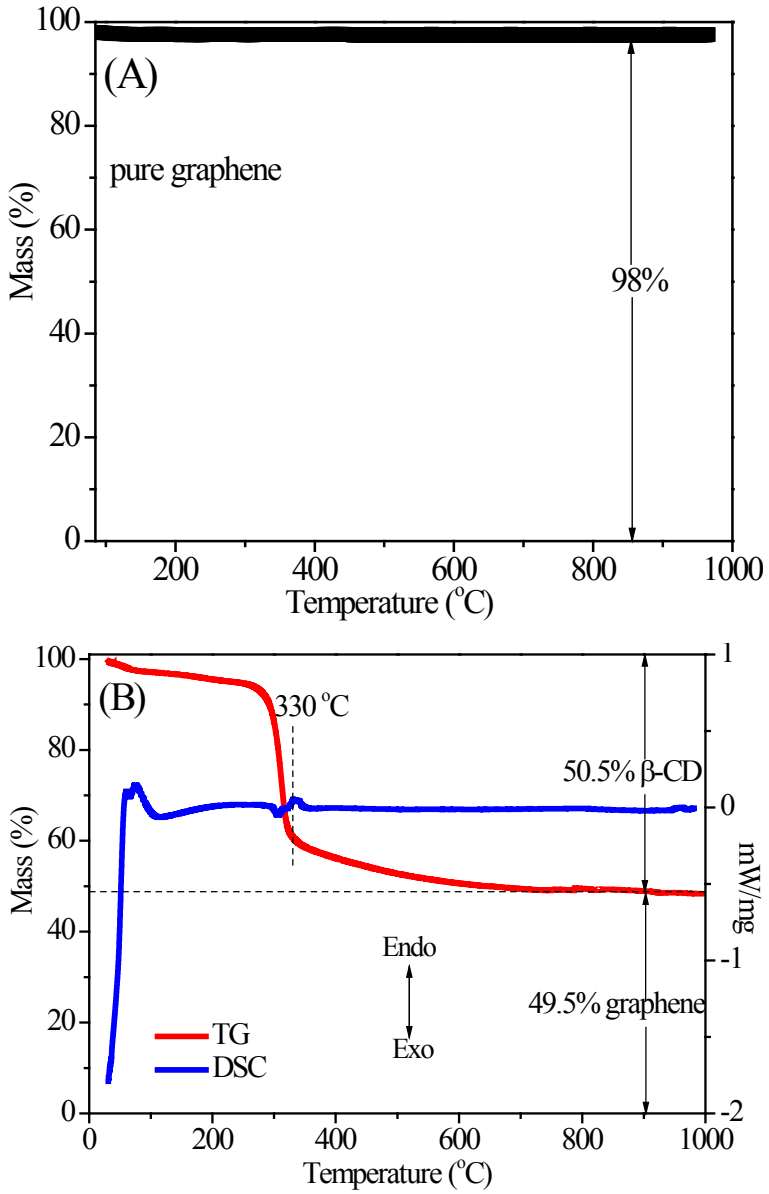

Figure S3. TG curves of pure graphene (A) and sample b (B).

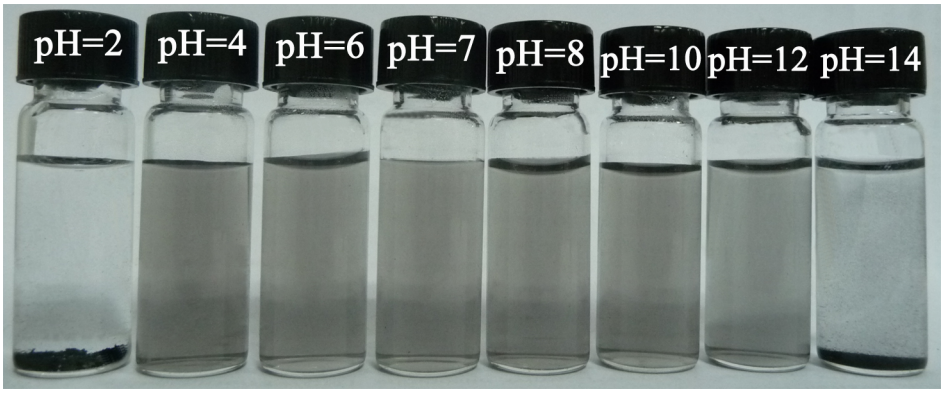

Figure S4. Optical micrographs of the dispersibility of β-CD/graphene composites dispersed in H_2O at pH values from 2 to 14. (c = 0.1 mg mL^{-1})