Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Efficiency of solvents and intercalators for exfoliation

Table S1 Minimum kinetic energy required for exfoliation (four different solvents).

Model	Minimum kinetic energy (kcal/mol)
Ethanol	16000
THF	14000
DMF	12000
NMP	10000

Table S2 Minimum kinetic energy required for exfoliation (four different intercalators).

Model	Minimum kinetic energy (kcal/mol)
Anthracene	9000
2-ACA	7000
2,3-ADCA	6000
2,6-ADCA	5000

Effect of an amine functionalization

2-aminoanthracene (2-AA) was used as an intercalator in the NMP solvent. The GO-intercalator interaction energy and the dipole moment of the 2-AA were calculated in the insertion simulation. The GO-intercalator interaction energy was shown as 2-ACA > 2-AA > Anthracene. The dipole moment difference between the GO sheets and the intercalators was shown as Anthracene > 2-AA > 2-ACA. This reveals that adding the amine functional groups on the anthracene can improve the exfoliation performance of the anthracene with the GO-anthracene interaction. However, the effect of the carboxyl functional groups on the exfoliation performance of the anthracene is larger than that of the amine functional groups.

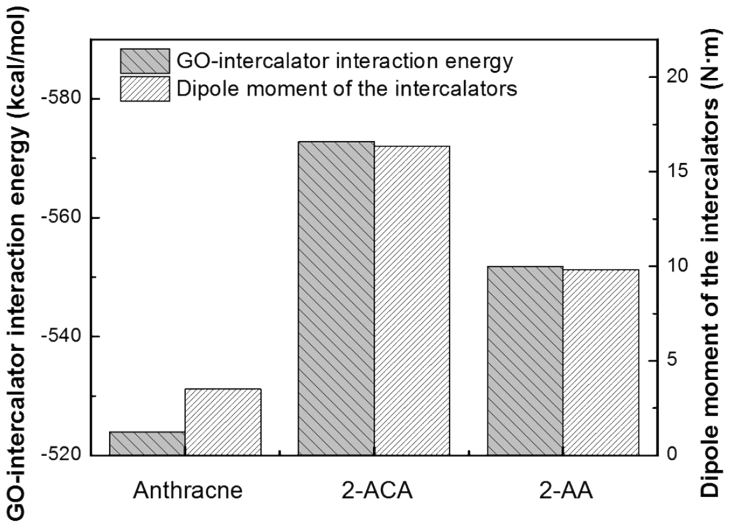

Fig. S1 A GO-intercalator interaction energy and the dipole moment of the intercalators: anthracene, 2-anthracenecarboxyl acid (2-ACA), and 2-aminoanthracene (2-AA).

A graphite exfoliation using carboxyl functionalized intercalators

A molecular model of the graphite was made by stacking five graphene sheets. The NMP solvent molecules was dispersed around graphene sheets. The six carboxyl functionalized intercalators (2,6-anthracenedicarboxylic acid; 2,6-ADCA) were used as the insertion molecule. In the insertion simulation, the kinetic energy of the insertion molecules increased with uniform incremental of 1000 kcal/mol from zero. Fig. S2 shows the Graphene-Graphene interaction energy with respect to the kinetic energy of the intercalators. The red dotted line indicates the beginning point of exfoliation. The red symbol is the minimum kinetic energy required for exfoliation. The minimum kinetic energy required for the graphite exfoliation was 9000 kcal/mol. In addition, the interaction energy between the graphite and the 2,6-ADCA molecules was -524 kcal/mol.

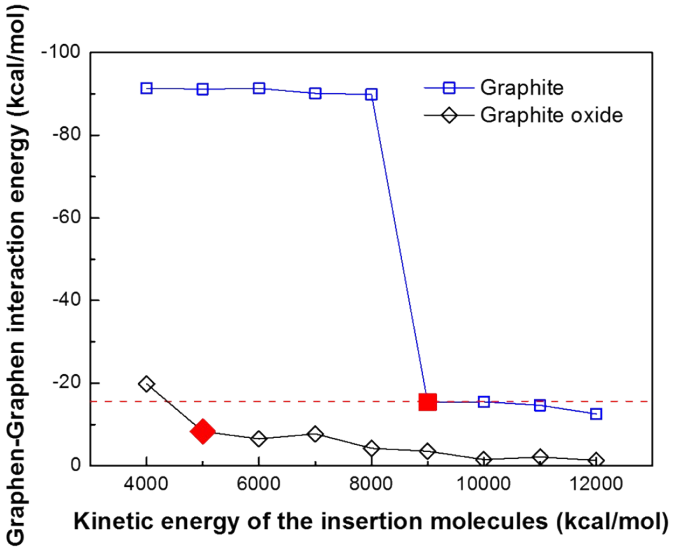

Fig. S2 A graphene-graphene interaction energy with respect to the kinetic energy of the intercalators.