RSC Advances

Supporting Information

Dielectric Environment as a Factor to Enhance the Production Yield of Solvent Exfoliated Graphene

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S1. Calculation of Mass fraction and yield of graphene

Further, thickness of the graphene layers was used to quantify the number fractions, mass fractions and overall yield of graphene layers obtained from different graphene based dispersions. We have calculated the mass fraction of graphene which is defined as[4]

$$\frac{M_{mono}}{M_{all}} = \frac{\sum_{individual} A_{mono}}{\sum_{all} N_{mono} A_{mono}} \quad (1)$$

where, A_{mono} is the area of monolayer and N_{mono} represents the number of monolayers in a given flake. The mass fraction of graphene monolayers obtained using fresh dispersions has been found to be between 3.4 wt % - 16.6 wt % in various solvents (Table I). Mass fraction of graphene monolayers can be used to calculate the overall yield using relation[4]

$$Y = \left(\frac{M_{mono}}{M_{all}} \right) \times \delta \quad (2)$$

where δ is the remaining fraction of sediment after centrifugation.

S 2.0 Electronic structure calculations:

Previously, DFT was used to understand, how different organic molecule are interacting with the graphene sheets and whether charge are transferred from graphene sheets to molecule or vice-versa. Calculations were carried out using DFT with Lee-Yang-Parr correlation

functional (B3LYP), with 631G-basis set. It has been observed that a p-type (n-type) graphene can be obtained, via charge transfer from graphene (organic molecule) to organic molecules (graphene)[1-2]. The charge transfer interms of Mulliken charge was calculated and it was noticed that, for low *k* solvent, a charge transfer of 0.0086e from graphene to organic molecule and for high *k* a charge transfer of 0.0365e from organic molecule to graphene was found. It corroborates the *n*-type (*p*-type) doping in graphene layers prepared in high-*k* (low-*k*) solvents.

Table I. *Summary of the statistics generated by analyzing large no. of AFM images of graphene layers obtained by exfoliation of HOPG in various solvents along with their respective surface energies. (Data corresponds to sonication time of 12 hours).*

Solvents used for exfoliation	Surface energy (mJ/m^2)	Total no. of flakes imaged	No. of monolayers	Size of graphene mono layers (μm)	No.of multilayers	No. fraction of Mono layer graphene (%)	Mass fraction of mono layer graphene (wt %)	Fraction of material (δ) remaining after centrifugation (%)	Overall yield (wt %)
Toluene	59	30	5	5-10	25	16	10.06	3.3	0.38
Chlorobenzene	64	25	4	7-10	21	16	11.4	3.8	0.47
Acetone	55	20	3	7-10	17	15	16.8	4.8	0.67
Acetonitrile	60	12	3	5-6	9	25	14	6.9	0.96
DMF	68	25	6	5	19	24	13.9	7.1	0.97
PC	71	30	8	8-12	22	25	16.5	7.4	1.28

References.

[1] M. Chi, Y. P. Zhao, *Computational Materials Science* 2012, **56**, 79.

[2] T. Hu, I. C. Gerber, *J. Phys. Chem. C* 2013, **117**, 2411.