Supplementary Material (ESI) for RSC Advances

Electronic Supplement for: Investigation of Graphene Oxide Nanosheets Dispersion in Water Based on Solubility Parameter: A Molecular Dynamics Simulation Study

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To justify the validity of the potential we used in this work, the structural parameters and density of single layer GO were compared with those calculated using DFT quantum mechanics, ReaxFF,[1] and other theoretical and experimental studies. As described in the text, the quantum mechanics DFT calculations in B3LYP/6-31G (d) level of theory, were done to obtain the optimized structural parameters and to extract the initial partial atomic charges. All DFT calculations were performed using Gaussian 09 program package. The optimized structure of GO is presented in Fig. 1. We also performed a MD simulation on a single layer GO (3×3 nm^2) using ReaxFF. It is worthy to mention that the high computational cost for ReaxFF (especially for multilayer GO and GO/water mixed system) hindered us to use this force field.[2] The MD simulation was done using ReaxFF at *NPT* ensemble of 300 K and 1 bar. All of simulation conditions are the same (time step, total simulation time, thermostat, and barostat). Table S1 shows the structural parameters obtained with different methods and it compares them to those obtained using our applied force field and other theoretical and experimental methods. Table S1 indicates that there is a good agreement between different mean bonds lengths obtained using force field employed in this work with those obtained using various methods. The maximum

difference belongs to hydrogen bond (H–bond) length calculated using our force field (1.98 Å) and that obtained using ReaxFF (1.75 Å). From this Table it is clear that our H–bond length (1.98 Å) is in consistent with those obtained using DFT quantum mechanics. Furthermore, density calculated using our force field is in excellent agreement with that calculated using ReaxFF.

Table S1. Justification of validity of potential used in this work.

Property	Mean bond length (Å)			
	Our force field	ReaxFF	DFT [a]	Theory or Exp.
C–C	1.50	1.47	1.48-1.52	1.51[3], 1.48-1.53[4], 1.54[5]
C=C	1.38	1.35	1.36-1.38	1.36[4]
C–H	1.03	1.02	1.04	0.97[6]
C–O	1.43	1.44	1.43-1.47	1.43-1.48[4], 1.44[5], 1.42-1.44[6]
C=O	1.32	1.30	1.22-1.23	1.22-1.23[6]
O–H	0.99	0.97	0.98	1.00[4]
O --- H (H–bond)	1.98	1.75	1.79-2.01	1.95[4]
Density (g cm^{-3})	2.46	2.42		

[a] Calculated in B3LYP/6-31G (d) level of theory.

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