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Can Structured Mixed Solvents be Used for Graphene Exfoliation? ANDREW OYER, CHETAN HIRE, JAN-MICHAEL CARRILLO, ALEXANDRU ASANDEI, DOUGLAS ADAMSON, ANDREY DOBRYNIN, University of Connecticut — Using a combination of computational and experimental techniques we investigate graphene exfoliation and suspension in C6H6, C6F6 and their mixtures. Our MD simulations show that an equimolar mixture of C6H6/C6F6 has the highest affinity for graphene. This is manifested in the formation of translational and orientational order normal to the graphene surface, with no translational ordering parallel to the graphene surface. The solvent structure is driven by quadrupolar interactions and consists of stacks of alternating C6H6/C6F6 molecules rising from the surface of the graphene. These stacks give rise to density oscillations in registry with the graphene surface. The period of the density oscillations is on the order of 3.4 Å, corresponding to the van der Waals diameter of carbon and this ordered structure extends 30 Å from each side of the graphene sheet. To experimentally verify the results of the molecular dynamics simulations we use dynamic contact angle measurements. These measurements demonstrate an increase in solvent affinity for HOPG in the case of 1:1 mixtures in comparison with pure components. The quality of the exfoliated material and flakes after sonication is verified by AFM, SEM, and TEM techniques. The graphene sheets produced in the equimolar mixture can be freeze-dried at room temperature, (T=300K) producing sponge-like graphene structures held together entirely by graphene sheet interactions and reflecting the structure of the graphene sheets in solution.

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