Understanding the role of molecular structure of the solvents in liquid phase exfoliation of two-dimensional materials

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Abstract

Obtaining 2D nanosheets and their dispersion through Liquid phase exfoliation (LPE) has gained significant attraction due to its various advantages. However, LPE requires a rigorous solvent selection procedure, and in this regard, several selection theories have been proposed over the past few years. Among them, the most widely accepted theory governing the solvent selection process is the Hansen solubility parameter (HSP). Although in the literature, it is observed that 2D dispersions in the solvents with similar HSP have different exfoliation efficiencies, to the best of our knowledge, the observed discrepancies with respect to HSP have not been accounted for. In this context, considering the large anisotropy of these materials, we have investigated the role of the molecular structure of the solvents having similar HSP in the LPE process using h-BN and $MoSe_2$ as 2D materials. It is observed that all five solvents chosen for the experiments possessed different exfoliation efficiencies contrary to our expectations from HSP theory, even when the same input exfoliation energies were imparted to the system. Further, the long-term stability of the dispersion was assessed using an analytical centrifuge employing STEP technology®. Although the HSP of the solvents are of similar values, the dispersion stabilities are different in different solvents. It is to note that these solvents are of different viscosity, which might play a crucial role in dispersion stabilization. The current experiments indicate that the low viscous solvent has better exfoliation efficiency and dispersion stability than the higher viscous solvent. Furthermore, there is no clear exfoliation trend according to the molecular sizes of the solvents, as proposed earlier in the literature. Therefore, based on the observed experimental results, we believe that molecular structure and the interaction between the solvents and the 2D nanosheets with mono or-a few-layer structures may have a critical role in LPE.

Figures

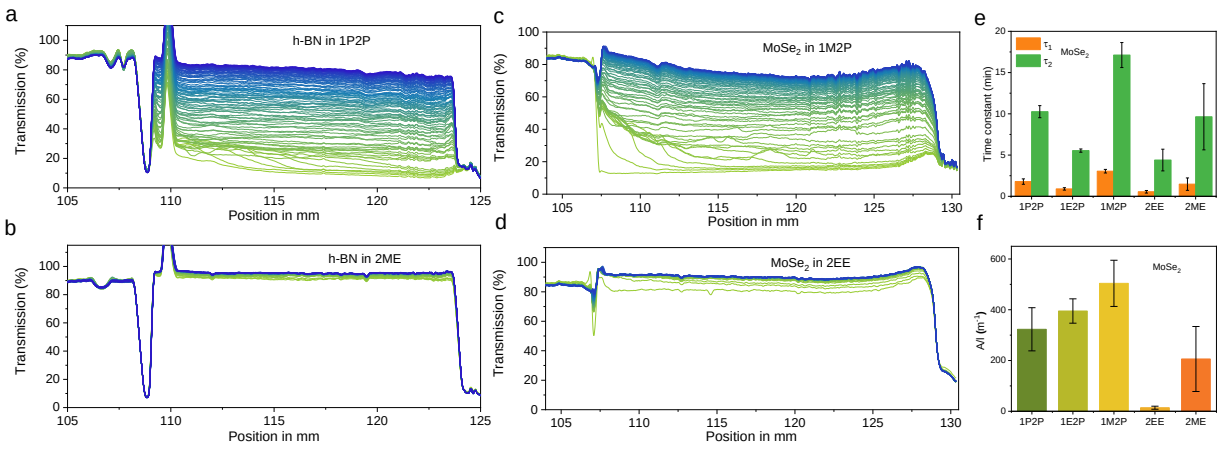

Figure 1: Dispersion stability of h-BN (a,b) and $MoSe_2$ (c-e) in best and worst solvents analysed using accelerated centrifuge. (f) Absorbance (A/I) of $MoSe_2$ dispersions at A-excitonic peak. Abbreviation: 2-methoxy ethanol (2ME), 2-ethoxy ethanol (2EE), 1-methoxy 2-propanol (1M2P), 1-ethoxy 2-propanol (1E2P) and 1-propoxy 2-propanol (1P2P).