Proceedings of the Canadian Society for Mechanical Engineering International Congress 2022
CSME Congress 2022
June 5-8, 2022, Edmonton, AB, Canada

New Insight into Liquid Phase Exfoliation of Graphitic Carbon Nitrides by Molecular Dynamics Simulations

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ABSTRACT

Graphitic carbon nitride (g-C_3N_4), as an intriguing conjugated polymer, has attracted broad attention due to its appealing electronic band structure, high physicochemical stability, and earth-abundant nature. It has been explored as a promising candidate in many applications such as photocatalysis, membrane, sensing, imaging, and energy conversion. Liquid phase exfoliation is the best-known method for the synthesis of two-dimensional (2D) g-C_3N_4 nanosheets. There have been a lot of experimental studies that aim at finding the promising solvents for efficient liquid phase exfoliation. However, the trial-and-error nature of these work do not allow for the molecular-level understanding of the process or novel design of effective solvents. Herein, we study the liquid phase exfoliation of g-C_3N_4 sheets in a number of solvents (aqueous and organic) using molecular dynamics (MD) simulations. To simulate the exfoliation process, potential of mean force (PMF) calculations were performed for the separation of two stacked g-C_3N_4 nanosheets, using umbrella sampling and the weighted histogram analysis method. The most probable path for the exfoliation process was identified. The impact of the solvent on the performance of the exfoliation was investigated by considering several intrinsic properties of the solvents, including their functional group, size, ability to form hydrogen bond, and solvation energy. Comparisons were made with existing experimental results, while the simulations generated additional mechanistic insights not accessible by experiments due to the lack of atomic resolution. Our findings provide a new framework for determining a solvent's performance in liquid phase exfoliation of 2D materials.