Summary of PhD Thesis - by Moyassar Meshhal

on

“Computational Perspectives on Environmental Applications of Two-dimensional Materials”

The escalating environmental challenges of our era demand innovative solutions, and 2D materials emerge as promising candidates with remarkable properties and tunability across diverse applications. This thesis explores the potential of harnessing 2D materials for environmental remediation through three comprehensive case studies.

The first investigation delves into the intricacies of water diffusion confined between graphene oxide (GO) layers, utilizing extended tight-binding (xTB)-based molecular dynamics simulations. Emphasis is placed on the impact of inter-layer H-bonded bridges, revealing novel insights into slowing down water diffusion. These findings not only hold implications for membrane technology but also offer a fresh perspective on selectively permitting species' movement for applications in selective separation processes.

The second case study investigates the behavior of hydrophobic and hydrophilic polymers, including polystyrene, polyethylene, and polyethylene oxide, at the graphene/water interface. Analysis of polymer dynamics uncovers graphene's ability to adsorb polymers, showcasing promise for the effective removal of nanoplastics from aqueous environments. This study not only calls for further exploration of the dynamics of polymers and water at the proximity of graphene and other 2D materials but also introduces valuable insights into understanding the adsorption capacities of graphene and graphene-based 2D materials.

In the third case study, the focus shifts to the potential of antimonene to capture the highly toxic organic molecule, 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD). DFT calculations demonstrate the promising capability of antimonene in adsorbing TCDD, with the exploration of different dopants revealing improved performance. These findings not only open avenues for optimizing antimonene properties but also underscore the nuanced effects of doping on the material's capturing capabilities.

Collectively, these case studies contribute to our understanding of 2D materials in environmental remediation, introducing novel insights into water diffusion, polymer adsorption, and toxic molecules capture. The interconnected nature of these studies underscores their potential impact on membrane technology, environmental remediation, and tailored materials design for adsorption purposes. This work marks initial steps towards practical applications, emphasizing the importance of interdisciplinary collaborations and the potential significance of these findings for addressing broader environmental challenges.