Computational modeling of modified 2D materials with deep eutectic solvents for water contaminant removal

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Abstract

The widespread presence of contaminants such as heavy metals, dyes, PFAS, pharmaceuticals, and pesticides in the aquatic environment poses a significant threat to public health and ecological balance. This work introduces a novel approach to water treatment technology, focusing on the computational modeling of two-dimensional (2D) materials, including graphene (Gr), graphene oxide (GO), and reduced graphene oxide (rGO) modified with natural deep eutectic solvents (NADESs) for effective contaminant removal. The study used Density Functional Theory (DFT) calculations and COSMO-RS analysis to evaluate the affinity and selectivity of these 2D materials and NADESs for various contaminants. The results showed that GO exhibited a significantly higher affinity for a broad range of pollutants compared to Gr and rGO, suggesting its superior potential in water purification. Additionally, among the tested NADESs, thymol-based DES demonstrated the best performance in enhancing the removal of contaminants. The findings underscore the promise of 2D materials and NADESs in developing sustainable, efficient water treatment technologies. These results provide a strong foundation for future experimental work and the development of novel materials that can be applied in various applications, such as membrane fabrication, adsorption, catalysis, and sensor development, all designed to improve the removal efficiency of a wide range of contaminants from water.

References

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Figures

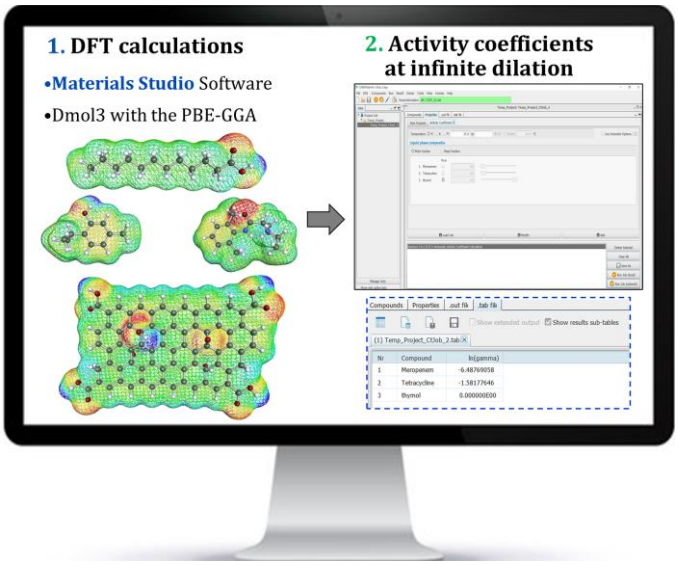

Figure 1: Quantum chemical calculations for 2D materials modified deep eutectic solvents.