A First-Principles Approach for Treating Dye Wastewater

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Abstract

Numerous materials are employed for treating wastewaters, e.g., for the removal of dyes from wastewater in the textile industry. However, the regeneration/reuse of these materials is still seldom practiced. Quantitative insights into intermolecular forces between the contaminants and the functional surfaces might aid the rational design of reusable materials. Here, we compare the efficacies of aliphatic (C8H18), aromatic (C6H6), and aromatic perfluorinated (C6F6) moieties at removing methylene blue (MB+), as a surrogate dye, from water. We employed DFT with an implicit water model (PCM) to accurately determine the contributions of the solvent's electrostatics in the adsorption process. These calculations pinpointed the relative contributions of π-π stacking, van der Waals complexation, hydrogen bonding, and cation-π interactions. QM predicted that MB+ would bind the strongest with C6F6 due to hydrogen bonding and the weakest with C8H18. Laboratory experiments revealed that despite the similar hydrophobicity of silica beads functionalized with Si-C8H17, Si-C6H5, and Si-C6F5, as characterized by similar water contact angles, the relative uptake of aqueous MB+ varied as Si-C6F5 (95%) > Si-C6H5 (35%) > Si-C8H17 (3%). This first-principles-led experimental approach can be extended to other classes of dyes, and it should advance the rational design of adsorbents for treating wastewaters.

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