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Adsorption of molecules on graphene: A semiempirical, empirical and DFT calculation approach.

Two active fields in the post-graphene era concern with molecular self-assembly at surfaces and the chemical exfoliation of graphite. As both processes are microscopically driven by the strength of the interaction with graphene, predicting the adsorption energy accurately and from first principles is attracting increasing interest. Here, the adsorption energy of a series of chemically diverse compounds on graphene has been evaluated using a wide range of methods at different levels of theory, from empirical Force Field (FF) to Semiempirical Quantum Mechanics (SQM) and Density Functional Theory (DFT). The results of the calculations are compared with literature Temperature Programmed thermal Desorption (TPD) experiments. We find that both the empirical and the semiempirical methods yield adsorption energies in good agreement with experiments with an average error of < 3 kcal/mol. We conclude that the use of these computationally less intensive methods provides the best compromise for the investigation of 2D self-assembly or the chemical design of novel graphene exfoliators.