Exploring the performance of graphene-based materials for pesticide removal from water: A DFT and COSMO-RS approach

Nesrine Kherra[1], Ammar Mosbah [2], Hakim Baaziz [2, 3], Tarek Lemaoui [4], Inas M. AlNashef [4, *]

[1] Department of Physics, Faculty of Science, Université Ferhat Abbas, 19000, Sétif, **Algeria**
[2]Department of Physics, Faculty of Science, University of M'sila, 28000, M'sila, **Algeria**
[3]Laboratory of Physics and Chemistry of Materials, University of M'sila, M'sila, **Algeria**
[4]Department of Chemical and Petroleum Engineering, Khalifa University,
P.O. Box 127788, Abu Dhabi, **United Arab Emirates (UAE)**

nesrine.kherra@ku.ac.ae

The growing issue of water systems caused by pesticides poses a significant environmental and health challenge. This study investigates the potential of graphene-based materials, including graphene (Gr), graphene oxide (GO), and reduced graphene oxide (rGO), as effective adsorbents for pesticide removal from water. The density functional theory (DFT) and COSMO-RS approaches were applied to examine the interaction between graphene-based materials and various pesticide molecules, including insecticides, rodenticides, miticides, fungicides, and herbicides Family. The results emphasize the superior adsorption performance of GO due to its abundant functional groups, enabling strong interactions through hydrogen bonding and van der Waals forces. The findings suggest that graphene-based materials, particularly GO, offer a promising solution for enhancing the efficiency of pesticide removal, contributing to sustainable and advanced water treatment technologies. The implication of this work lays the groundwork for future studies on optimizing graphene-based adsorbents for large-scale environmental applications.

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Figures

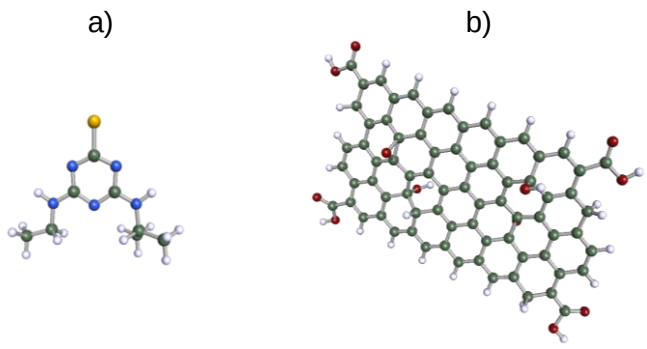

Figure 1: 2D molecular structures: a) atrazine and b) graphene oxide.