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The role of defects in graphene for removal of toxic compounds

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Understanding the adsorption of pesticides and toxic gases on graphene has high importance for their degradation and removal. In the present study, the adsorption of different models of organophosphate pesticides (OPH3, OPF3, SPH3 and SPF3) on perfect and defected graphene was examined by using the DFT method. Inspected systems were pristine, single-vacancy (SV), Stone-Wales (SW) and epoxy graphene. Pristine graphene exhibits great adsorption affinity towards OPH3 molecule, while it shows insignificant adsorption towards other examined species. The introduction of defects influences the reactivity of these molecules on the graphene surface. Among them, SV graphene showed the highest adsorption affinity for OPH3 and OPF3, while SW graphene showed the most suitable adsorption properties towards SPH3 and SPF3 molecules. The interaction between molecules and graphene was mostly physisorption except in the case of epoxy graphene where degradation of organophosphates occurred. This study suggests that graphene can be potentially used to remove environmental pollutants and pesticides' chemical degradation, while the surface chemistry of graphene should be carefully tailored for this application.

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