Physical Chemistry Student Seminar

“Computational Investigations of Organic Reactions on Graphene, Fullerenes and Carbon Nanotubes”

In the past thirty years, carbon-based nanomaterials, including fullerenes, carbon nanotubes and graphene, have spurred great interest due to their unique physical and chemical properties. Fullerenes and carbon nanotubes have been well studied, while studies of graphene, a relatively new material, are less advanced. A variety of chemical modification strategies have been successfully established on fullerenes and carbon nanotubes, and important functional changes have been demonstrated. Some attempts have been made to transfer these chemical modifications onto more inert graphene, yet very few give satisfactory results. I will describe density functional theory calculations to study one of the functionalization approaches, cycloaddition reactions, on carbon allotropes, especially graphene. Ideally graphene is composed solely of sp2 carbons in extended conjugation. These extended π systems can function either as 2π or 4π components in cycloaddition reactions. We have explored 1,3-dipolar cycloadditions, Diels-Alder reactions, (2+2) cycloadditions, (4+4) cycloadditions and (1+2) cycloadditions on a series of graphene models. We also assessed non-covalent interactions of aromatics and small π system with graphene. Our work provides clear predictions of the energetics of the adduct formation on different sites of graphene, increasing understanding of graphene chemistry and guiding experiments carried out by collaborators.

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12:00 P.M.

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