

**Energetics of Adsorption of Monocyclic Carbon Rings on Graphene:
Distance and Orientation Dependence from Analytical Approaches**

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Small carbon clusters have received tremendous attention from both theoretical and experimental communities in recent years because of their important role in hydrocarbon flames, astrochemistry and formation of fullerenes. Theoretical studies have revealed that the most stable structures for carbon clusters with 10, 12, 14, 16, 18, 20 and 22 carbon atoms are monocyclic rings.¹ However, experimental production and isolation of carbon rings is extremely difficult due to their high reactivity. Therefore, herein, we address the following questions: (1) Can adsorption on graphene serve as a strategy for the isolation of monocyclic carbon rings? (2) What are the energetics for the adsorption of various rings on graphene? In this work, the energetics for the adsorption process are investigated using the analytical approaches, developed earlier by James M. Hill and co-workers.^{2,3,4} The adsorption process is driven by the non-covalent interactions between the carbon ring and the graphene sheet. The study comprises both the continuum and the discrete-continuum models. The analyses of the interaction energy as a function of both the vertical distance Z and the rotational angle ϕ are done in order to determine the preferred orientations, equilibrium positions and binding energies for the adsorption of various carbon rings on the graphene sheet. We find that the preferred orientation of the rings with respect to the graphene sheet is parallel.⁵ The analytical models employed by us are computationally cheap, can provide important insights into the adsorption process and can serve as starting points for high level quantum chemical calculations.

References:

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