**Carbon-Based Nanosheet: Pioneering Approaches for Organic Pollutants Adsorption**

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**Abstract:**

This research focuses on studying the way benzophenone derivatives (BP-1, BP-2, and BP-3) interact with graphene oxide (GO) surfaces using density functional theory (DFT). The study involved optimizing the structures of the GO adsorbent, benzophenone derivatives, and their complexes through computational calculations. The analysis revealed that the interaction between the GO surface and the adsorbates is physically-based. The adsorption process was found to be spontaneous, exothermic, and irreversible, as indicated by the calculated values of adsorption energy, Gibbs free energy (ΔGad), and enthalpy (ΔHad). The stability of the studied structures was confirmed by negative values of the calculated chemical potential. The adsorption of BP pollutants onto the GO surface resulted in increased dipole moments compared to the unadsorbed molecules. The efficiency of adsorption followed the trend GO-BP-2 > GO-BP-3 > GO-BP-1. Furthermore, infrared (IR) frequency calculations confirmed the validity of the structures. The results from Natural Bond Orbital (NBO) and Frontier Molecular Orbital (FMO) analyses indicated that GO is an effective adsorbent for removing organic BP pollutants from water. The study also considered various parameters related to the adsorption behavior, including charge capacity, electrophilicity, band gap, chemical potential, and chemical hardness. In summary, this study employed computational methods to investigate the adsorption behavior of BP derivatives on GO surfaces, providing valuable insights into their thermodynamics, stability, and effectiveness as adsorbents.

**Biography of Presenter about 100 words:**

Dr. Foad Buazar is a highly accomplished professional with a distinguished academic background and expertise in the field of Chemistry. He holds a PhD degree in Organic Chemistry from Tarbiat Modares University, Iran, which he earned in 2009. Recognized as one of the world's top 2% scientists by Stanford University, Dr. Buazar has made significant contributions to the field of green nanochemistry, particularly in the areas of environmental remediation, organic synthesis, and modeling.

With a focus on the treatment of water and wastewater's organic contaminants, Dr. Buazar's primary research revolves around the synthesis of eco-friendly nanoparticles and organic catalysis. His current endeavors are exploring innovative approaches, such as photocatalytic degradation of emerging pollutants using environmentally friendly organic and inorganic nanomaterials.

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