A First-Principles Examination of Hydrogenated Graphene in the Context of Artificial Molecules

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The remarkable mechanical, optical, and electronic properties of graphene have fueled research in various domains, including energy storage, energy conversion, spintronics, and semiconductor applications. A key aspect of graphene's versatility is its ability to be functionalized through surface adsorption, which modifies both its geometric and electronic characteristics. Such functionalization suggests that graphene could serve as a "quantum simulator platform," enabling the realization of otherwise unstable molecular structures. In this work, we employed density functional theory calculations to investigate monolayer graphene with adsorbed hydrogen atoms. By examining three distinct adsorption configurations—ortho, meta, and para—we identified the para-type arrangement as the most stable configuration. Additionally, we propose that selectively positioning adsorption sites could facilitate the formation of isolated artificial molecules. Our findings lay the groundwork for exploring unstable molecular species and offer valuable insights into their fundamental properties.