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INSIGHTS ON METAL DOPED GRAPHENE IN THE ADSORPTION OF ARSENIC VIA A DFT CALCULATION

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Abstract. Arsenic contamination in drinking water poses significant health risks worldwide, making the development of efficient removal technologies a critical area of research. This study explores the enhancement of graphene's arsenic (As) adsorption capabilities through metal doping at various positions on its surface. Using density functional theory (DFT), the interactions between arsenic and graphene doped with selected metals were simulated, evaluating the influence of different doping positions on adsorption efficiency. The results demonstrate that metal doping significantly improves the arsenic removal capacity of graphene, with variations observed depending on the doping configuration. These findings contribute to a deeper understanding of the adsorption mechanisms in graphene-based materials and offer a computational approach for designing advanced adsorbents for environmental remediation.

Keywords: adsorption, modeling, density functional theory, 2D material, metal doping effect, graphene, molecular simulation.