# Impact of Protonation on the Adsorption Properties of Phenols on Graphene Oxide: Insights from DFT Calculations

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With the rapid advancement of industrialization, a wide array of carbon-based and inorganic materials is increasingly used in essential sectors such as petrochemicals, textile dyeing, coal industry, polymer production, biopharmaceuticals, and process engineering. These manufacturing processes frequently result in the generation of polluted water, containing complex constituents—such as heavy metals, dyes, pesticides, phenolic compounds . . . —that are often non-degradable or challenging to break down, posing significant risks to toxicity and environmental health. Phenolic compounds are often overlooked, yet their discharge can severely harm aquatic life, soil, and overall ecosystems, posing risks to health. Currently, various methods—such as organic carbon adsorption, advanced oxidation processes, membrane-based techniques, and reverse osmosis—are employed to remove carbon-based contaminants from polluted water. However, the stability of phenolic pollutants presents significant challenges, making these decomposition methods not only lengthy and costly but also prone to by-product formation. In recent decades, adsorption treatment has emerged as a preferred approach due to its operational simplicity and cost-effectiveness. Among the various adsorption strategies, the use of nanomaterials, particularly graphene oxide (GO), has gained significant attention for its effectiveness in pollutant removal [2]. Graphene oxide is a versatile nanomaterial known for its high surface area, abundant functional groups, and remarkable adsorption properties. These characteristics enable GO to effectively capture a wide range of contaminants, including phenolic compounds, thereby providing a promising solution for water treatment applications. In addition to experimental methods, computational simulation techniques are utilized to investigate and clarify the entire reaction process at the molecular level. In this study, we systematically explore the interactions between various phenolic compounds commonly present in wastewater, including phenol, 2,4-dichlorophenol, p-cresol, pentachlorophenol, 4-(2,4-dimethylheptan-3-yl)phenol, 4-nitrophenol, bisphenol A, and 2-chlorophenol, and their adhesion to graphene oxide. Our primary objective is to analyze the variations in adsorption energy, adsorption distance, and electron density distribution when neutral or protonated phenolic compounds interact with graphene oxide, utilizing first-principles calculations. Additionally, Reduced Density Gradient (RDG) analysis enables us to examine both strong and weak van der Waals interactions—both repulsive and attractive—between phenolic compounds and the graphene oxide surface. This comprehensive analysis allows us to assess distinct adsorption behaviours effectively. The findings of this research indicate a promising strategy for the removal of phenolic pollutants from wastewater.

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## References

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