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Computational Studies of Transition-Metal Decorated Graphene Adsorbent for Air Pollutants Removal

Coal combustion in a coal power plant is a major source causing severe environmental implication such as releasing elemental mercury (Hg0), toxic arsine gas(AsH3), and volatile organic compounds (VOCs) into the atmosphere. In this work, we have investigated transition metal decorated graphene as adsorbent for removal of these pollutants from flue gas using density functional theory calculation on three applications. In the first application, boron-doped graphene decorated with transition metal nanocluster(M-BDG) is used to study the adsorption of Hg0 (for M = Pd, Pt, Ru, W). The result shows that Pd4-BDG is the most efficient adsorbent for Hg0 adsorption, while capacity investigation suggests that maximum of 6 Hg atoms per Pd4 site can be adsorbed via chemisorption. In the second application, Pd nanocluster is deposited on single-vacancy graphene (SDG) for AsH3 adsorption. The study reveals the size effect of Pd cluster on the adsorption strength of AsH3 and its variants based dominantly on Coulomb interaction. In the third application, transition metal nanocluster decorated SDG is used to study adsorption selectivity of heterocyclic VOCs on various metal species. The result shows that organonitorgen compound adsorbed the strongest among all VOCs, especially on Pt4 (-2.11 eV). In conclusion, computational insights from our studies provide key understandings for enhancement of graphene-based adsorbent design and synthesis.

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