THE EFFECT OF pH ON THE U(VI) SORPTION ON GRAPHENE OXIDIES: A THEORETICAL STUDY

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Along with the development of nuclear power, radioactive waste water has become one of the world’s great environmental challenges, which is also a hot spot in scientific research. In addition to the numerous experimental researches, quantum chemical calculations are a new and viable complement to experiments in addressing various problems related to the nuclear chemistry. At present, the pollution of radioactive U(VI) can be a serious threat to the public health and ecosystem stability; and the graphene oxides (GOs) can be used for the removal of uranium from radioactive wastewater. In present work, by means of high-level computational calculations, we scrutinized the detailed geometric structures and the adsorption energies for different GOs uranyl complexes at various pH values. 13 adducts of GOs uranyl complexes were optimized by applying density functional theory (DFT) method together with the PCM model in which the solvent effect was considered. To exploring the bonding structure between the U(VI) and GO-based materials, 3 oxygen-containing functional groups (epoxy oxygen, hydroxyl group, and carboxyl group) were used in this study. By analyzing the adsorption energy and the structures of different adducts, we can conclude that the uranyl ions prefer to be bound to the anionic GO, that is, high pH is more favorable for the adsorption process of uranyl species on graphene oxides. And compared to the other forms of graphene oxide, the GO containing double hydroxyl groups has the highest adsorption capacity towards the uranyl species. The results construct a bridge interconnecting the experimental observations and the intrinsic mechanisms, which may bring new insight into the radioactive environmental pollution management.
Figure 1. The optimized structures of GO/uranyl complexes at different pH values.

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REFERENCES