Structural Design and Stability Simulation of Polymer Sponge for TBP and Dodecane Separation in Liquid Waste

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1. Introduction

As organic liquid waste, one of the hardly disposable radioactive wastes, has not been established for its treatment technology, the waste is temporarily stored in the research organizations or facilities. Although the use of incineration technology is known to be effective for the treatment of organic radioactive wastes, it is not possible for the general public to accept the environmental pollutants such as process corrosion and dioxin generated during the high temperature incineration process.[1] Alternative oxidation technologies (AOTs) have been developed since the 1980s to improve various incineration processes. Typical incineration alternatives include catalytic chemical decomposition processes, direct chemical decomposition, oxygenation, steam reforming, gas phase reduction, and a method for the oxidation of hydrochloric acid.[2]

However, despite the long-term research of these treatment methods, about 14 tons of organic radioactive waste, including TBP, dodecane, cutting oil, waste oil, alcohol, and etc., which were generated during the operation of the research institute, were temporarily stored in the Radioactive Waste Disposal Facility (RWTF) at Korea Atomic Energy Research Institute (KAERI). Therefore, in order to treat these radioactive liquid wastes, we have recommended the treatment method using a sponge filter made of polymer or graphene which have micro- and macro-pores completely different from the conventional treatment methods. If the organic compounds can be separated from the organic radioactive wastes, it is possible to effectively treat the organic radioactive wastes with minimization of further occurring radwastes.

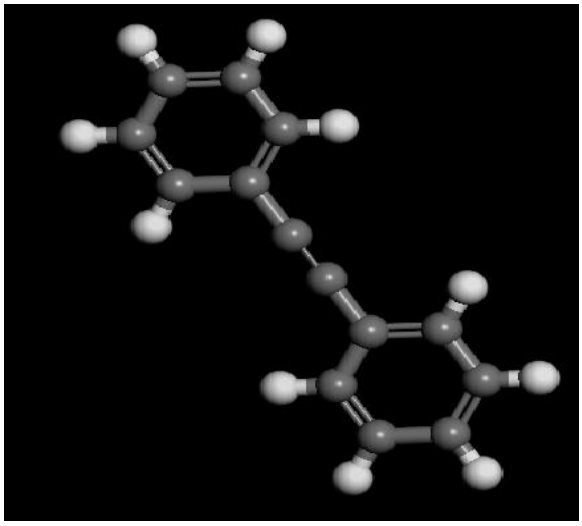

Fig. 1. Molecular structure of designed polymer sponge material.

2. Polymer Sponge Design

To selectively adsorb organic compounds such as TBP and dodecane in liquid wastes, several candidates of polymer sponge materials were selected. Fig. 1 shows one of the selected molecular structure among the polymer sponge candidates. Various factors like large adsorption

capacity for TBP and dodecane compounds, hydrophobicity, structural stability and etc. are considered in this polymer sponge.

3. Structural Simulation

In order to understand the structure and characteristics of synthesized candidates, Density of state (DOS), Bandstructure and Optimized structure were calculated by using Density Functional Theory (DFT) calculation technique. As a result of the calculations, it was found that the most stable form of the polymer sponge composed of honeycomb structure among all the polymer sponge candidates was observed. The geometry optimization of the polymer sponge was conducted due to confirmation of structural stability and geometry energy of about 20 kcal/mol after 40 calculation cycles was obtained (Fig. 2).

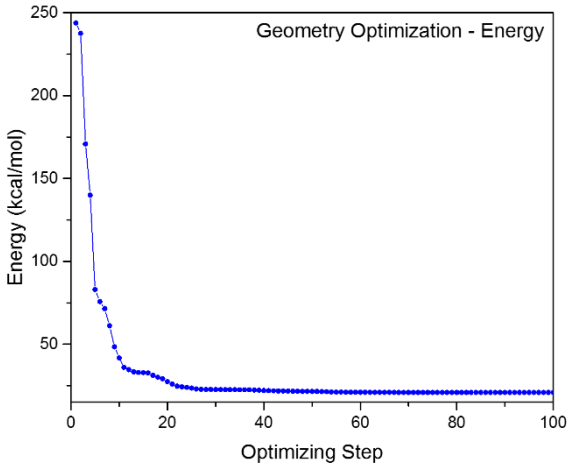

Fig. 2. Geometry energy optimization of designed polymer sponge material.

4. Conclusions

Through this study, a structure model of the polymer sponge is designed and its structural stability can be demonstrated by using DFT calculation. The structure of polymer sponge, which is expected to be the most stable among other candidates, has a honeycomb structure and it has a geometry energy of 20 kcal/mol which is quiet low. The results of this research will provide important information for designing the most efficient and stable polymer sponge materials in the theoretical way, and will be able to transmit the key factors for the treatment of organic liquid wastes when using the polymer sponge materials.

REFERENCES

[1] K.-W. Lee, H.-B. Yang and S.-H. Na, “Development of Technology of Advanced Oxidation Process (AOP) for Radioactive Organic Wastes”, KAERI Research Report (2012).

[2] D.-Y. Chung and et al., “Development of technologies for treatment of decommissioning wastes”, KAERI Research Report (2017).