A study for development a porous materials to extract alkanes from radioactive liquid wastes

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1. Introduction

At the Korea Atomic Energy Research Institute (KAERI), organic radioactive waste contaminated with radionuclides has been generated through various research activities. The organic radioactive wastes contain acetone, alcohol, tributyl phosphate (TBP), dodecane and so on.

The amount of organic radioactive waste is small compared to aqueous radioactive waste, but effective management strategies for such waste are needed to ensure safe handling, treatment, storage and disposal. Aqueous radioactive wastes may be released to the environment after the radioactivity has decayed or been removed, while, organic radioactive wastes need management steps that not only take account of their radioactivity, but also of their chemical effect. This is because both the radioactivity and the organic chemical content can have detrimental effects on health and the environment.

Various methods of treating organic radioactive waste, such as incineration or wet oxidation, have been developed, but there are also problems with each treatment method, such as the generation of corrosive gases generated after incineration and secondary wastes generated from other methods.

If the organic matter and the inorganic matter can be separated from the organic radioactive waste, it is possible to effectively treat the organic radioactive waste using the evaporation concentrate and the natural evaporation treatment technique, and the amount of the organic waste can be drastically reduced.

In this study, two polymeric compound candidates capable of selectively adsorbing only organic materials in the mixed solution were selected and the structural safety and adsorption ability of the materials were obtained by computer simulation

2. Methods and Results

Two building blocks were prepared as candidate materials to extract alkanes. Fig. 1 shows the building block 1 and 2 which are used in this study.

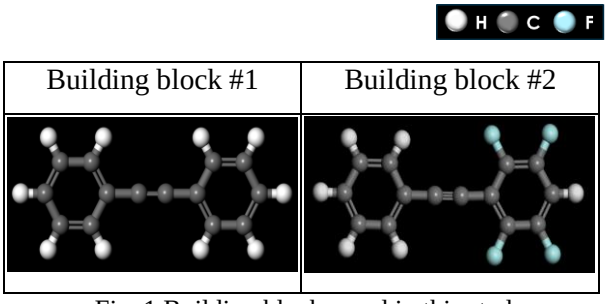
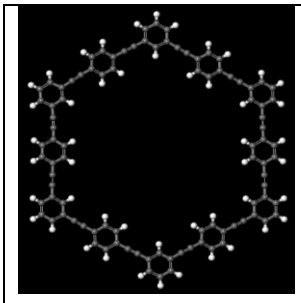


Fig. 1 Building blocks used in this study

Total energy of optimized structure and binding energy between candidate structure and dodecane was calculated using Density Functional Theory (DFT) [1] calculation technique. DFT calculations were performed using DMol3 code, which is widely used worldwide.

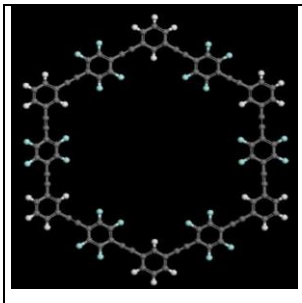
2.1 Structure stability

The structure stability calculation were performed using geometry optimization calculation. The structure energies for building block #1 and #2 are -538.9445Ha and -935.7220Ha, respectively. Using each building block, we made hexagonal structure like honeycomb which is considered as most stable structure. The structure energy result of dodecane is 527.5545Ha. Fig 2 and 3 show the total energy of building block #1 and as honeycomb structure with dodecane, respectively.



(a)	(b)
Total E : -3683.1248Ha	Total E -4155.5703Ha

Fig. 2 Geometry calculation results for (a) hexagonal building block #1 (b) with dodecane



(a)	(b)
Total E : -6063.7440 Ha	Total E -6536.1842 Ha

Fig. 3. Geometry calculation results for (a) hexagonal building block #2 (b) with dodecane

Analysis of the final energy of the structure including dodecane shows that the energy of -472.4434Ha and -26.9947Ha is lower than the sum of the energy of the honeycomb structure and the energy of dodecane in building blocks 1 and 2, respectively. The details are summarized in Fig 4 and 5 for each building block.

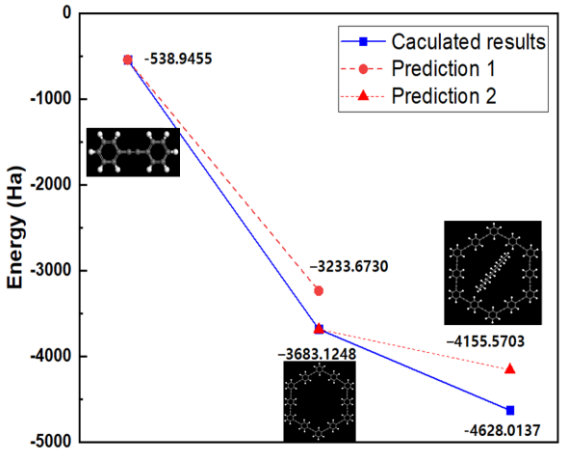


Fig. 4. The tendency of structure stability calculation for building block #1.

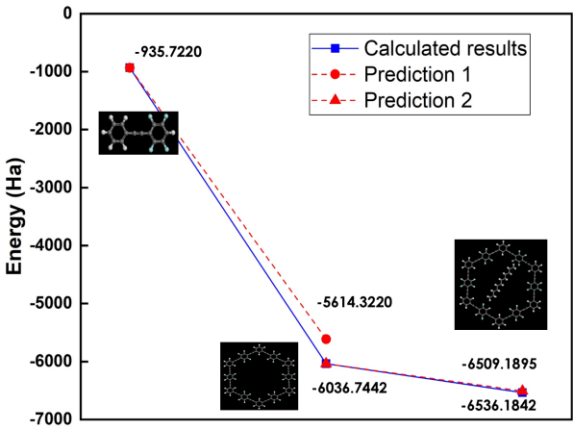


Fig. 5. The tendency of structure stability calculation for building block #2.

As a result, it was found that polymer compounds composed of honeycomb structures of all the candidate polymer compounds were obtained in the most stable form, and that actual synthesis was possible.

2.2 Absorption

In order to calculate the absorption ability to dodecane, binding energy calculation was performed. Table 1. Summarized the results for the binding energy between dodecane and candidate building blocks.

Table. 1. Results of binding energy between dodecane and candidate building blocks

Building Block	#1	#2
Biding E (Ha)	-0.0387	-0.0091
Biding E (Ev)	-1.05	-0.25

The adsorption energy of the organic material was found to be lower than the adsorption energy of some hydrogen substituted fluorine structures.

3. Conclusions

Structure stability and binding energy were calculated using DMol3 Module which is a general DFT calculation module. The structure stability with dedecane of building block #1 is more stable than that of building block #2, and the binding energy of #1 is also higher than building block #2.

According to the results, it can be consider that #1 building block is optimized candidates of polymer-sponge materials that can separate organic compounds and inorganic waste liquid by dodecane in organic liquid radwaste. More than 3~4 building blocks would be further investigated.

4. References

[1] Hohenberg, P. and Kohn, W: Pysical Review B, **136,** pp 864-871 (1964)