

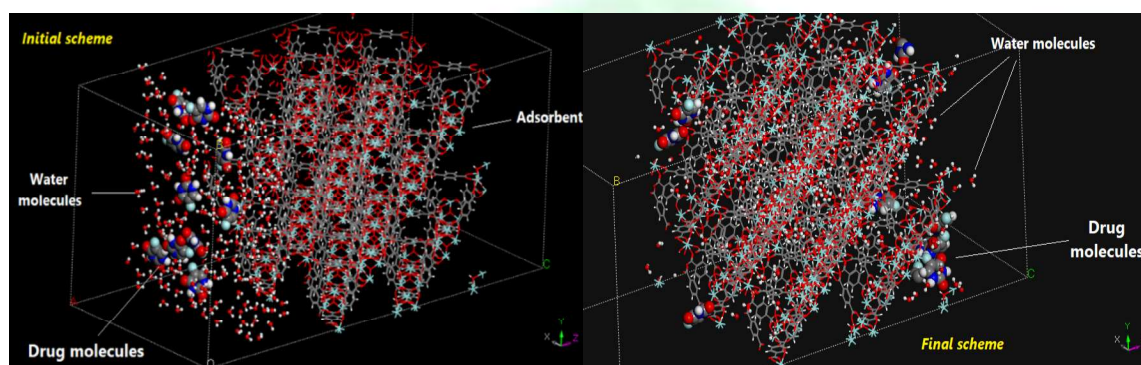
Biocompatible Adsorbent for Drug Storage and Removal Applications: A Molecular Dynamics Study

M. Akbari, F. Moosavi*

Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, 9177948974, Islamic Republic of Iran

*Email: moosavibaigi@um.ac.ir

Graphical Abstract



Abstract: Water pollutants can be classified as many kinds such as organics and inorganics that mainly are discharged from industrial effluents and human sewage into the water [1]. Metal Organic Frameworks (MOFs) have been used widely as molecular adsorbent due to their large surface area, high pore volume, high payload, low toxicity and biocompatibility [2-3]. MOF drug delivery system (DDS) can prevent drug release into the water by restricting the drugs into MOFs. In addition, DDS can also reduce the side effects of anticancer drugs while they circulate into the body [4]; MOFs can be used as filters [5]. In this study, we investigated two anticancer drugs, 5-fluorouracil (5-FU) and gemcitabine (GEM), diffusion and storage into UiO-66 by molecular dynamic (MD) simulations. In order to gauge diffusion of 5-FU and GEM into UiO-66, mean square displacement (MSD) was computed for both promising drugs. MD simulations show an acceptable adsorption and diffusion of 5-Fu in MOF unlike GEM drug. Adsorption of GEM was



10th National Biennial Seminar (Webinar) of Chemistry and Environment



mostly on exterior sites of UiO-66 due to high diameter of GEM than the diameter of UiO-66 pores.

References

- [1] K. L. Wasewar, S. Singh, and S. K. Kansal, Chapter 13 - Process intensification of treatment of inorganic water pollutants, in *Inorganic Pollutants in Water*, Editors: P. Devi, P. Singh, and S.K. Kansal, Elsevier, pp. 245-271, **2020**.
- [2] I. Erucar, and S. Keskin, *Journal of Materials Chemistry B*, vol. 5, pp. 7342-7351, **2017**.
- [3] M. Kotzabasaki, and G. E. Froudakis, *Inorganic Chemistry Frontiers*, vol. 5, pp. 1255-1272 **2018**.
- [4] C. Jeyaseelan, P. Jain, D. Soin, and D. Gupta, *Inorganic and Nano-Metal Chemistry*, vol. 51, pp. 1-13. **2021**.
- [5] M. Kadhom, and B. Deng, *Applied Materials Today*, vol. 11, pp. 219-230, **2018**.