

A theoretical and experimental study of adsorbent dye removal from (2E, 5E)-2,5-Bis(4-methoxybenzylidene) cyclopentanone using diatomaceous earth as an adsorbent

Veprim Thaçi^{1,2,3}

Rilinda Plakaj¹; Ardhmeri Aliaj¹; Arianit Reka⁴; Jane Bogdanov³; Ramiz Hoti¹; Avni Berisha^{1,2}

¹ Department of Chemistry, Faculty of Natural and Mathematical Science, University of Prishtina "Hasan Prishtina" George Bush, 10000 Prishtina, Republic of Kosova

² Academy of Science of Albania, Unit of Albanian Nanoscience and Nanotechnology - NanoAlb, 1000 Tirana, Albania

³ University of Skopje "Ss. Cyril and Methodius" Institute of Chemistry, blvd. Goce Delcev 9, 1000 Skopje, Republic of North Macedonia Republic of North Macedonia

⁴ Department of Chemistry, Faculty of Natural and Mathematical Science, University of Tetovo. Str. Ilinden, nn. 1200 Tetova, Republic of North Macedonia

veprim.thaci@uni-pr.edu

This study is focused on the adsorption of (2E,5E)-2,5-Bis(4-methoxybenzylidene) cyclopentanone using diatomaceous earth. First, the monocarbonyl compound was synthesized, then crystallized and characterized was done with IR, NMR, etc. The theoretical calculations based on Density Functional Theory (DFT) and Monte Carlo (MC) calculations were used to explore the preferable adsorption site, interaction type, and adsorption energy of the (2E,5E)-2,5-Bis(4-methoxybenzylidene) cyclopentanone onto diatomaceous earth.

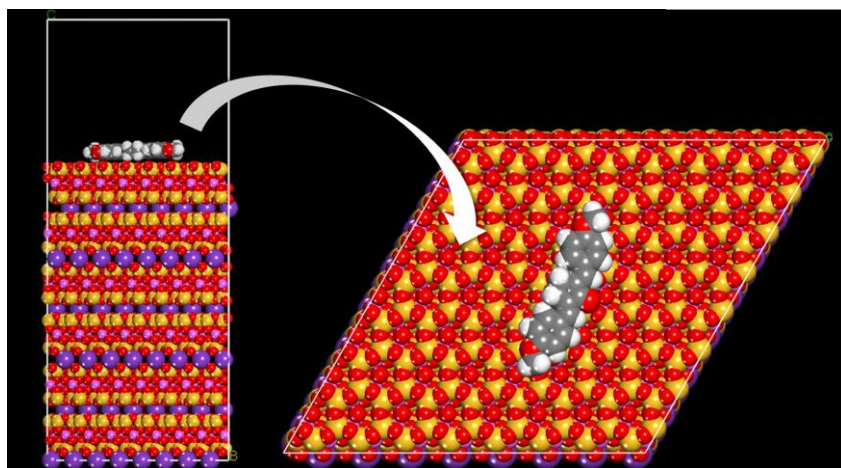


Figure 1: Monte Carlo lowest energy geometry obtained during the adsorption of the adsorption of the 2E, 5E)-2,5-Bis(4-methoxybenzylidene) cyclopentanone using diatomaceous earth modelled using Muscovite structure (Amcsd 0000854).

Diatomaceous earth soil is cleaned, homogenized and characterized by various spectroscopic methods and is used as an adsorbent. The adsorptive ability of the diatomaceous earth toward the (2E, 5E)-2,5-Bis(4-methoxybenzylidene)cyclopentanone was evaluated using UV-Vis measurements.

Keywords: MACs; adsorbent; theoretical calculation; NMR; synthesis.

References

- [1] Ardhmeri Aliaj, Drinisa Gashi, Rilinda Plakaj, Admir Omaj, Veprim Thaçi, Arianit Reka, Sefer Avdiaj, Avni Berisha*. A theoretical and experimental study of the adsorptive removal of hexavalent chromium ions using graphene oxide as an adsorbent. *Open Chemistry* 2020; 18: 936–942. <https://doi.org/10.1515/chem-2020-0148>.
- [2] Shehdeh Jodeh, Ahlam Jaber, Ghadir Hanbali, Younes Massad, Zaki S. Safi, Smaail Radi, Valbonë Mehmeti, Avni Berisha, Said Tighadouini & Omar Dagdag. Experimental and theoretical study for removal of trimethoprim from wastewater using organically modified silica with pyrazole-3-carbaldehyde bridged to copper ions. Jodeh et al. *BMC Chemistry* (2022) 16:17 <https://doi.org/10.1186/s13065-022-00814-0>.