

# Accepted Manuscript

Full Length Article

Selective Adsorption of Organic Dyes on Graphene Oxide: Theoretical and Experimental Analysis

Aniruddha Molla, Yuanyuan Li, Bikash Mandal, Sung Gu Kang, Seung Hyun Hur, Jin Suk Chung

PII: S0169-4332(18)32473-5  
DOI: <https://doi.org/10.1016/j.apsusc.2018.09.056>  
Reference: APSUSC 40360

To appear in: *Applied Surface Science*

Received Date: 26 June 2018  
Revised Date: 9 August 2018  
Accepted Date: 6 September 2018

Please cite this article as: A. Molla, Y. Li, B. Mandal, S. Gu Kang, S. Hyun Hur, J. Suk Chung, Selective Adsorption of Organic Dyes on Graphene Oxide: Theoretical and Experimental Analysis, *Applied Surface Science* (2018), doi: <https://doi.org/10.1016/j.apsusc.2018.09.056>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



# Selective Adsorption of Organic Dyes on Graphene Oxide: Theoretical and Experimental Analysis

Aniruddha Molla, Yuanyuan Li, Bikash Mandal, Sung Gu Kang, Seung Hyun Hur, Jin Suk Chung\*

School of Chemical Engineering, University of Ulsan, Namgu, Daehakro 93, Ulsan 680-749, South Korea.

Email: jschung@mail.ulsan.ac.kr (J. S. Chung)

**Abstract:** The adsorption behaviors of methylene blue, rhodamine B, and methyl orange over graphene oxide were studied both experimentally and theoretically. From the experimental results and characterizations of fresh graphene oxide and graphene oxide after adsorption, selective adsorption of positive dye occurred via electrostatic interactions between the  $=N^+H$  group (positive dipole from dye molecules, MB) and oxygen functional group of GO (negative dipole), as identified in the zeta potential, FT-IR, and XPS analyses. The selectivity for positive dye was rapid and quantitative where removal efficiencies of 97% and 88% were obtained for the positive dyes methylene blue and rhodamine B, respectively, within 15 min; the negative dye, methyl orange, was not adsorbed. The most probable arrangement of dyes on graphene oxide was evaluated using Ab initio molecular dynamics, and the adsorption energy was calculated. The most favorable adsorption configuration was found at 2,298 fs for methyl orange and 2,290 fs for methylene blue. Our results demonstrate that methylene blue is more strongly (-2.25 eV/molecule) adsorbed on the GO surface than methyl orange (-1.45 eV/molecule).

**Keywords:** Graphene oxide, Organic dyes, Selective adsorption, Ab initio molecular dynamics.

Download English Version:

<https://daneshyari.com/en/article/9569557>

Download Persian Version:

<https://daneshyari.com/article/9569557>

[Daneshyari.com](https://daneshyari.com)