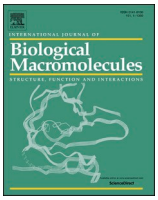
International Journal of Biological Macromolecules 242 (2023) 124798



Contents lists available at ScienceDirect

International Journal of Biological Macromolecules

journal homepage: www.elsevier.com/locate/ijbiomac





Fabrication of chitosan@activated carbon composites in EmimAc for Cd(II) adsorption from aqueous solution: Experimental, optimization and DFT study

Ismaila Olalekan Saheed [a,b], Enis Nadia Md Yusof [c], Wen-Da Oh [a], Megat Ahmad Kamal Megat Hanafiah [d], Faiz Bukhari Mohd Suah [a,*]

[a] Green Analytical Chemistry Laboratory, School of Chemical Sciences, Universiti Sains Malaysia, 11800 Minden, Pulau Pinang, Malaysia
[b] Department of Chemistry and Industrial Chemistry, Kwara State University, Malete, P.M.B 1530 Ilorin, Nigeria
[c] Chemistry Section, School of Distance Education, Universiti Sains Malaysia, 11800 Minden, Pulau Pinang, Malaysia
[d] Faculty of Applied Sciences, Universiti Teknologi Mara, Cawangan Pahang, Lintasan Semarak, 26400 Jengka, Pahang, Malaysia

ARTICLE INFO

Keywords:
1-ethyl-3-methylimidazolium acetate
Activated carbon
Adsorption
Cd(II)
Chitosan composites
Ionic liquid

ABSTRACT

Adsorption efficiency of a duo-material blend featuring the fabrication of modified chitosan adsorbents (powder (C-emimAc), bead (CB-emimAc) and sponge (CS-emimAc)) for the removal of Cd(II) from aqueous solution was investigated. The chitosan@activated carbon (Ch/AC) blend was developed in a green ionic solvent, 1-ethyl-3-methyl imidazolium acetate (EmimAc) and its characteristics was examined using FTIR, SEM, EDX, BET and TGA. The possible mechanism of interaction between the composites and Cd(II) was also predicted using the density functional theory (DFT) analysis. The interactions of various blend forms (C-emimAc, CB-emimAc and CS-emimAc) with Cd(II) gave better adsorption at pH 6. The composites also present excellent chemical stability in both acidic and basic conditions. The monolayer adsorption capacities obtained (under the condition 20 mg/L [Cd], adsorbent dosage 5 mg, contact time 1 h) for the CB-emimAc (84.75 mg/g) > C-emimAc (72.99 mg/g) > CS-emimAc (55.25 mg/g), as this was supported by their order of increasing BET surface area (CB-emimAc (120.1 m^2/g) > C-emimAc (67.4 m^2/g) > CS-emimAc (35.3 m^2/g)). The feasible adsorption interactions between Cd(II) and Ch/AC occurs through the O−H and N−H groups of the composites, as supported by DFT analysis in which an electrostatic interactions was predicted as the dominant force. The interaction energy (−1309.35 eV) calculated via DFT shows that the Ch/AC with amino (−NH) and hydroxyl (−OH) groups are more effective with four significant electrostatic interactions with the Cd(II) ion. The various form of Ch/AC composites developed in EmimAc possess good adsorption capacity and stability for the adsorption Cd(II).

1. Introduction

In recent times, modern technology has led to the release of large amounts of hazardous heavy metals into the aquatic environment. Heavy metals are toxic, non-degradable with a tendency of accumulating in the body of living organisms causing various illnesses and disorders such as cancer, renal damage, and kidney disorder [1]. Cadmium (Cd) is one of the toxic heavy metals utilised in variety of industrial processes and materials, which eventually finds its way into the aquatic environment as effluents. The World Health Organization has limited the amount of Cd in drinking water to 0.003 mg/L [2]. Therefore, Cd must be effectively removed from wastewater streams before discharging into the environment in order to guaranty a safer environmental health. Various methods such as chemical precipitation, ion exchange, electrochemical treatments, membrane technologies, photocatalysis, adsorption, have been utilised to remove this metal from wastewaters [3,4]. Conversely, adsorption is often preferred due to its simplicity, low energy consumption, relatively efficient and rapidness [5]. This has led to the quest for an excellent adsorbent for the removal of this contaminant.

Furthermore, several adsorbents such as biosorbents [6], natural materials [7], and waste materials from agricultural source and industries have been utilised for adsorption of pollutants from wastewater [8]. Some reported adsorbents for Cd include clay materials [4], zeolites

* Corresponding author.
E-mail address: fsuah@usm.my (F.B.M. Suah).

https://doi.org/10.1016/j.ijbiomac.2023.124798
Received 11 January 2023; Received in revised form 18 April 2023; Accepted 6 May 2023
Available online 11 May 2023
0141-8130/© 2023 Elsevier B.V. All rights reserved.