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Article

Interpretation of Adsorption Behavior of Carboxymethyl Cellulose onto Functionalized Accurel Polymeric Surface

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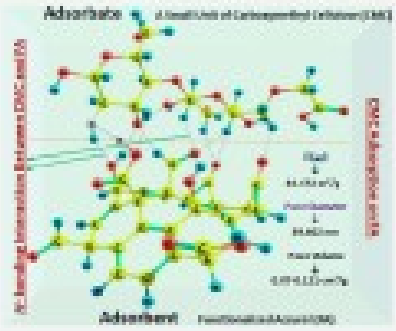
ABSTRACT: Carboxymethyl cellulose (CMC) is the most versatile cellulose derivative having several industrial applications such as mineral processing, pelletization process, oil drilling, surface modifications, functionalization of materials, and other promising utilizations. However, the less interpretation of the adsorption behavior of CMC onto the functionalized polymeric surface in its aqueous medium hinders its applications. The present contribution has, therefore, been made to explore the binding aspects of CMC onto functionalized accurel (FA) derived from polypropylene-based Accurel (MP1001). The physicochemical parameters of FA such as specific surface area (S_{BET}) = 34.472 m^2/g, pore volume (V_p) = 0.07−0.121 cm^3/g, total pore volume (V_p) = 0.115 cm^3/g, mean pore diameter = 13.692 nm, and pore diameter = 39.402 nm were determined by the Brunauer−Emmett−Teller (BET) analysis. The batch shaking adsorption experiments with various parameters were conducted, and the equilibrium isotherm data were fitted with the Freundlich, Langmuir, Temkin, and Jovanovic models of adsorption and compared by determination coefficient (R^2), which followed the order: Langmuir (R^2 = 0.9933) > Freundlich (R^2 = 0.9830) > Jovanovic (R^2 = 0.9428) > Temkin (R^2 = 0.8663). The infrared and X-ray photoelectron spectral changes before and after adsorption were recorded, which confirmed the hydrogen bonding between the carbonyl group of CMC and functional groups (−OH) of FA in the regions 288−280 eV and 1772−1676 cm^{-1}, respectively. To understand the type, nature, and strength of interaction(s) involved in the adsorbent−adsorbate complex (FA−CMC), a theoretical model is adopted in this report. With the deployment of the density functional theory (DFT) dispersion-corrected (DFT-D) and DFT approaches, geometric stability and electronic feature analyses have been performed using the optimized structure, binding/interaction energy, highest unoccupied molecular orbital−lowest unoccupied molecular orbital (HOMO−LUMO) gap, natural population analyses, and Bader's quantum theory of atoms in molecules (QTAIM)-based parameters. The reactive sites of the aforementioned species have been detected using the molecular electrostatic potential surface (MESP) map. The exhibition of different geometrical and electronic features including the binding aspects of the adsorbate CMC onto the polymeric surface of the adsorbent FA was exercised via CMC accumulation stabilized by H-bonding and other weak noncovalent interactions and since such alteration could play a noteworthy role in the fields of food, pharmaceutical, and industrial chemistry.



1. INTRODUCTION

Carboxymethyl cellulose (CMC) is a widely available cellulose derivative having various characteristic properties such as anionic water solubility, nontoxicity, biocompatibility, biodegradability, and naturally occurring polysaccharide. These characteristic properties of CMC are associated with the hydroxyl groups present in its structure. CMC has been extensively used in industrial areas including biopolymeric and nanopolymeric materials in various applications.[1−8] The applicability of CMC depends on the understanding of interfacial binding aspects (adsorption) onto polymeric/solid/mineral surfaces. The adsorption aspects were adopted by many researchers not only for understanding the CMC adsorption onto various surfaces but also in various environmental and pharmaceuticals studies. In these studies, the authors described the distribution of the various adsorbate species between liquid and several adsorbents through linearly plotted graphs based on a set of assumptions related to the heterogeneity or homogeneity of various adsorbents, surface coverage, and the different binding behaviors between the several adsorbates. Therefore, various adsorption models were adopted to describe and understand the present work.[9−11] The binding behavior of CMC is associated with its several commercial applications

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