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Atomic-scale interactions of the interface between chitosan and Fe_3O_4

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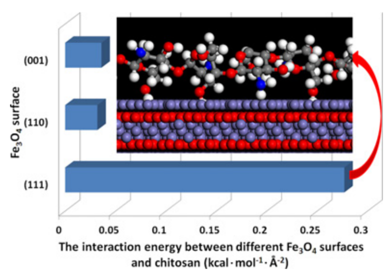
HIGHLIGHTS

- We built the interface model between chitosan and Fe_3O_4.
- The (1 1 1) interface has strongest interaction than other interfaces.
- There was high probability of formed hydrogen bonds of (1 1 1) interface.
- There were interactions between Fe_3O_4 and nitrogen atoms of chitosan.

GRAPHICAL ABSTRACT



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ABSTRACT

Molecular dynamics (MD) simulation was employed to study chitosan adsorption on different Fe_3O_4 crystallographic planes at the atomic level. The interaction energy between chitosan and different Fe_3O_4 surfaces indicates that the interaction of chitosan and Fe_3O_4 (1 1 1) surfaces is stronger than that of (1 1 0) and (0 0 1) surfaces. The concentration profiles show that hydrogen and amino groups of chitosan could form strong interactions with the surfaces of Fe_3O_4. The radial distribution function show that the probability of forming hydrogen bonds between groups of chitosan and oxygen atoms on Fe_3O_4 (1 1 1) surface is more than that of Fe_3O_4 (1 1 0) surface, and the nitrogen atoms and iron atoms on the surface have weak physical interactions. This study provides useful information in understanding the interfacial interaction mechanism at the atomistic scale for polymer and mineral.

1. Introduction

The iron oxide nanoparticles (Fe_3O_4 NPs) were a kind of important magnetic material. It has been widely used in bio-separation, hyperthermia and magnetic guided drug targeting [1–4]. For biomedical applications, Fe_3O_4 NPs were often treated by surface modification which could increase the functionality and improve the biocompatibility of the Fe_3O_4 NPs [5]. Chitosan obtained by deacetylation of chitin was a unique natural linear cationicpolymer, which was the structural element in the exoskeleton of crustaceans and cell walls of fungi. Chitosan had many beneficial properties such as a low toxicity, low immunogenicity, excellent biocompatibility, biodegradability and as well as a high positive charge density. Due to its high positive charge density, it could easily form polyelectrolyte complexes with negatively charged nucleotides or drugs by electrostatic interaction [6–8].

Recently, chitosan modified magnetic particles (MPs) have gained significant attention for biomedical applications. Li et al. has reported the MPs can provide excellent biocompatility, biodegradability and low toxicity without compromising their magnetic targeting [9]. Sun et al. have prepared magnetic targeting chitosan nanoparticles as a drug delivery system and imaging agents for photodynamic therapy to cancer treatment [10]. Nguyen and co-workers have developed a novel chitosan Fe_3O_4 nanobiocomposite-based platform for electrochemical detection of HIV-1 [11]. Although, MPs have applied in many fields, the

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