A Novel Approach to Prepare Hydroxyapatite/ Cellulose Nanocomposites by novel methods: DFT study, molecular docking, and in silico ADMET studies

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Abstract. This paper presents a novel cheminformatics approach for the design and synthesis of hydroxyapatite/cellulose nanocomposites, which have potential biomedical and environmental applications, removal of dyes. The nanocomposites are syn-thesized by the co-precipitation method with different ratios of hydroxyapatite and cellulose. Over the past decade, calcium phosphate composites and similar biomaterials have seen commercial use in bone substitution and allograft applications. These biomaterial composites, which include an organic matrix and an inorganic mineral, have been developed. The principal inorganic component is hydroxyapatite, with the organic matrix made of cellulose derived from Esparto "*STIPA TENACISSIMA* TENDRARA" which covers the territory of Tendrara, from Eastern- Morocco. The final product received extensive characterization using techniques such as FTIR, XRD, thermal analysis, Morphological studies, XPS, 31P NMR, AFM, SEM, Ligand preparation and Prediction of ADME/ Toxicity Properties, with SEM micrographs revealing the product's nanometric size (Figure1), XRD analysis show that a significant hydrogen bonding interaction between HAp and cellulose may have occurred as the cellulose peak intensity steadily decreased with HAp level. Concurrently, enterprises have been recorded discharging substantial amounts of methylene blue into natural water sources, raising worries about human health and ecosystems. Computational analysis revealed the compound's properties, revealing potential side effects and environmental risks. Toxicity tests have identified considerable hazards, particularly for cardiac problems, necessitating cautious use. Theoretical computations confirmed the composites' high contact strength, particularly when HAp, Ce, and HAp/Ce were deprotonated. These findings are consistent with experimental evidence. Theoretical calculations utilizing Monte Carlo (MC) and Molecular Dynamic (MD) simulation models revealed that the produced foams had an outstanding affinity for methylene blue, as shown by strongly negative adsorption energy values indicating strong interactions with adsorbate surfaces. Based on the calculated chemical hardness values for the adsorbent, adsorbate, and the complex system, it can be inferred that the adsorbent system demonstrates a higher level of hardness in comparison to the adsorbate.

Keywords: Composite; Biomaterials; Cellulose; Hydroxyapatite; Molecular Dynamic simulation; DFT, ADMET, Monte Carlo (MC)

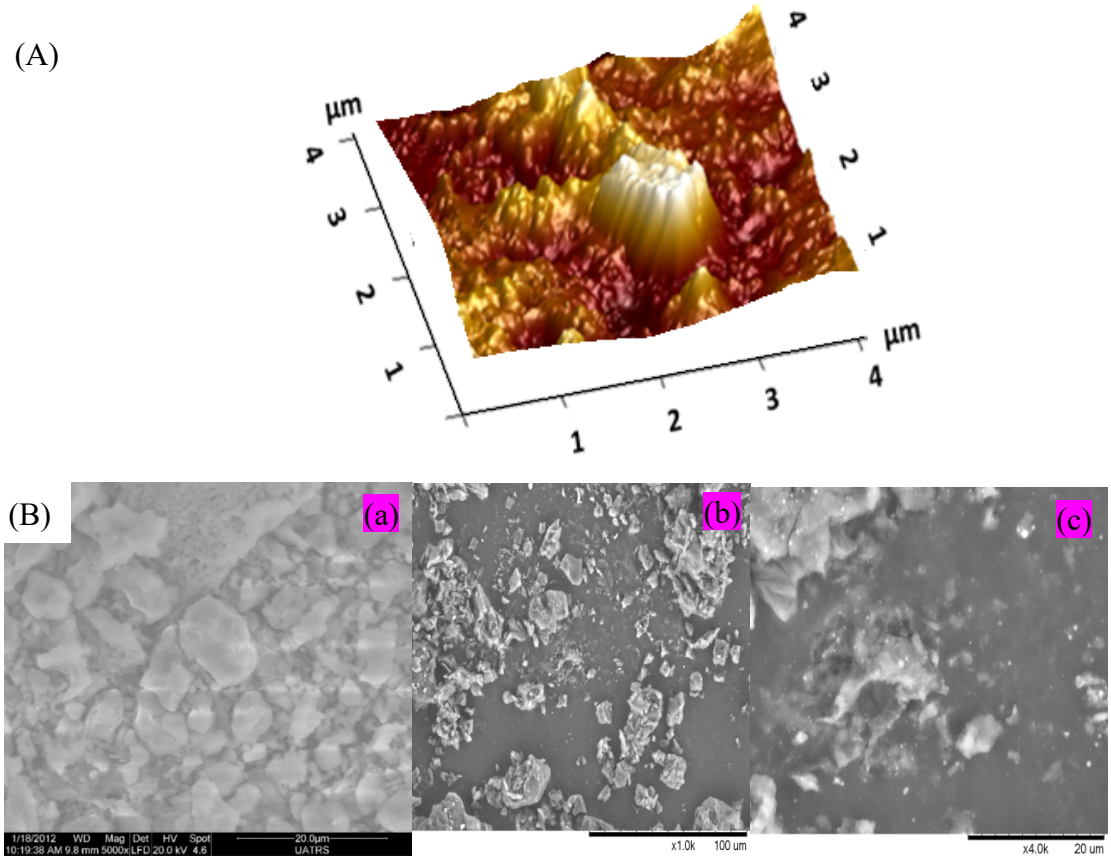

Figure 1. (A) AFM micrographs of mild steel surface in HAp/ Ce at 1 g / l, and **(B)** SEM/ FEG images of a: HAp, b: Ce and c: HAp/Ce composite.

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