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# **The removal of mercury ion pollution by using Fe<sub>3</sub>O<sub>4</sub>-nanocellulose: Synthesis, characterizations and DFT studies**

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## **Abstract**

In this study, we have attempted to extract cellulose from *Cystoseria myrica* algae. Nanocellulose, Fe<sub>3</sub>O<sub>4</sub> and Fe<sub>3</sub>O<sub>4</sub>-nanocellulose compounds are synthesized by acid hydrolysis and co-precipitation as well as sol-gel methods. The synthesized compounds are characterized by x-ray diffraction, transmission electron microscopy, particle size distribution (PSD), scanning electron microscopy (SEM), energy dispersive x-ray spectroscopy, vibrating sample magnetometer and Fourier transform infrared spectroscopy. The Hg (II) uptake on Fe<sub>3</sub>O<sub>4</sub>-nanocellulose is investigated by 14 isotherm models, 12 kinetic models, adsorption activation energy as well as thermodynamic of adsorption. The polymers of algae and the interactions between Hg (II) and cellulose are investigated by density functional theory (DFT) in various conditions. The results of both simulations show a good agreement with experimental data.

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