عنوان مقاله:

Removal of nickel (II) from aqueous solution by graphene and boron nitride nanosheets

محل انتشار:

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خلاصه مقاله:

Molecular dynamics simulations were carried out to study the removal of Ni2+ as a heavy metal from the water by the functionalized graphene nanosheet (GNS) and boron nitride nanosheet (BNNS). Nickel causes asthma, conjunctivitis and inflammatory reactions and nickel salts act as emetics when swallowed; therefore, removal of nickel is necessary from the aqueous solutions. The systems were comprised of a nanosheet (GNS or BNNS) with a pore in its center that it is containing an aqueous ionic solution of nickel chloride. For the removal of Ni2+ from an aqueous solution, the pores of nanosheet were functionalized by passivating each atom at the pores edge and then an external electric field was applied along the z-axis of the simulated system. To justify the passage of ions through the pores, the potential of the mean force (PMF) of ions was calculated. To evaluate the properties of the system, the ion retention time and the radial distribution functions of species were measured. Based on the findings of this study, these nanostructure membranes can be recommended as a model for removal of heavy metals

کلمات کلیدی:

Ni2+; GNS; BNNS; PMF; Heavy metal