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Computer modeling studies of the adsorption energies of heavy metals onto vermiculite surface

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Abstract content
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Computer modelling studies were performed to investigate the adsorption energies of selected heavy metal cations onto vermiculite (001) surface, using universal force field. The metal cations studied are Cu, Ni, Zn, Pb, Cd and Mn. The energies of the selected cations were negative showing that they are all miscible with vermiculite interlayer surface. The metals showed increasing adsorption energies in the following order: Cu < Ni < Zn < Pb in agreement with experimental findings. The other two metal cations, Cd and Mn, showed lower absorption energies contradicting experimental findings.

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