Tensor renormalization group study of simple lattice model of cation-anion binary adsorption layer on muscovite (001) surface

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Clays and clay minerals are widely used to extract heavy metals from soils due to their low cost, non-toxicity, and highly efficiency. Based on the literature data [1] [2], we have developed a simple lattice model of co-adsorption of metal cations and halogen anions from an aqueous medium on the muscovite (001) surface. The model describes the interaction of an aqueous salt solution with clay aluminosilicate material contained in the soil. The energies of lateral "cation-cation", "anion-anion" and "cation-anion" interactions are measured in relative values due to the general form of the model. We have analyzed the ground state (T = 0 K) of the lattice model. After that, this model was studied with the tensor renormalization group method at non-zero temperatures. The results obtained with tensor renormalization group method were compared with results of the grand canonical Monte Carlo simulations [3]. Features of the phase behavior of the system are revealed. Partial adsorption isotherms describing competitive adsorption of ions from aqueous salt solutions on the surface of muscovite were calculated. This study was supported by the Russian Science Foundation under Grant No. 22-71-10040.

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