Atomistic multiscale modeling of cement AFm phases

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AFm phases of cement, $[Ca_2Al(OH)_6]Cl_2H_2O$ (hydrocalumite) and $[Ca_2Al(OH)_6]I_2H_2O$, are considered as potential adsorbents for radioactive anions in the context of geological nuclear waste disposal. The Cl-containing phase has been studied quite extensively [1], while the experimental studies of the iodine-containing phase, have only been started [2]. We study the structure of AFm phases by density functional theory (DFT) calculations. For both systems DFT-D3 method with a combination of the Becke exchange functional and the LYP correlation potential (BLYP) were used. Also, we apply methods of classical molecular dynamics simulations via ClayFF-MOH force field [3] to quantitatively study the properties of these materials as potential adsorbents for radionuclides ^{36}Cl, ^{129}I, ^{137}Cs in their contact with CsCl aqueous solutions. Our results confirm and expand earlier atomistic simulations of hydrocalumite [1]. Also, we observe a weaker adsorption of I^-, compared to Cl-, and also a partial adsorption of Cs^+ cations. In addition, the diffusional mobility of surface-adsorbed ions significantly decreases compared to the bulk solutions. The research was conducted within the framework of the HSE University Basic Research Program. The calculations were performed on the supercomputer of HSE University.

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