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Radioactive Iodine-129 Capture in Mixed Cation Sodalites: ab initio modelling

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Sodalites have been investigated experimentally for the capture and long-term containment of iodine-129, a significant and hazardous waste product of the nuclear fuel cycle. Sodalites are zeolite-type structures commonly occurring in nature in alkaline igneous rocks and having the prototype formula $\text{Na}_8(\text{AlSiO}_4)_6\text{Cl}_2$. The crystal structure is based around β -cages consisting of corner-sharing SiO_4 and AlO_4 tetrahedra. In the centre of the β -cage is an anion X. Iodine captured by sodalites sits in the centre of the β -cages as iodide anions. Silver iodide (AgI) plays an important role in the capture and subsequent processing of iodine-129 in the nuclear fuel cycle. Using ab initio density functional theory (DFT) modelling, we investigate the energetics and feasibility of iodine capture and containment in mixed cation sodalites $\text{Na}_{8-x}\text{Ag}_x(\text{AlSiO}_4)_6\text{I}_2$, and compare the results with experimental observations.

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