

Formation of Volatile Iodine from Cesium Iodide Aerosols: A DFT Study

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Abstract : Periodic DFT calculations were performed to study the chemistry of CsI particles and the possible release of volatile iodine from CsI surfaces for nuclear safety interest. The results show that water adsorbs at low temperature associatively on the (011) surface of CsI, while water desorbs at higher temperatures. On the other hand, removing iodine species from the surface requires oxidizing the surface one time for each removed iodide atom. The activation energy of removing I_{2} from the surface in the presence of two OH is 1,2 eV.

Keywords : aerosols, CSI, reactivity, DFT, water adsorption

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