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MXene as Sorbent Materials for Off-gas Radioiodine Capture and Immobilization

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ABSTRACT:

The capture and further immobilization of the major regulated volatile radionuclides (such as ^{129}I and ^{85}Kr) from the off-gas streams of a used nuclear fuel (UNF) reprocessing facility has been a topic of significant research interest for the US Department of Energy (DOE) and other international colleagues. This proposal is focused on the development of MXenes as innovative sorbent materials for radioiodine capture and immobilization. MXenes have recently emerged as an intriguing family of graphene-like two-dimensional (2D) layer-structured transition metal carbides and/or nitrides with a high specific surface area, a tunable interlayer spacing, hydrophilicity, and abundant highly active surface sites. MXenes have the chemical formula $M_{n+1}X_nT_x$ (n is the number of carbides/nitrides octahedral blocks in each layer and it can be 1, 2, 3, or 4), where M represents early transition metals (Sc, Ti, V, Cr, Y, Zr, Nb, Mo, Hf, Ta, W), X represents carbon (C) and/or nitrogen (N), and T_x denotes surface groups such as -O, -OH, -F, and -Cl. MXenes do not have the disadvantage of weak van der Waals adsorption as they are composed of transition metal elements such as Ti and Nb, which confer excellent affinities toward heavy metals. Owing to the presence of abundant active sites terminated by numerous functional groups, MXenes not only provide sites for direct ion exchange but also effectively adsorb and immobilize radionuclides through chemical and electrostatic attraction. The interlayer spacing (d-spacing) of the layer-structured MXenes can be tuned through intercalation and/or exfoliation by using suitable intercalants, in such a way to encapsulate the radionuclides whose radii are larger than the layer d-spacing for MXenes with large adsorption capacities. Also, by widening the d-spacing, the interaction affinities of the surface anchored functional groups of MXenes with the radionuclides could be significantly improved as the layer d-spacing is a key factor influencing their ion exchange capacity. MXenes exhibit unique properties such as excellent chemical compatibility, high thermal stability, and good radiation resistance and offer the advantages of low-cost scalable production and high-yield on a laboratory scale, which make them to serve as ideal adsorbents for radionuclides including iodine based on various absorption mechanisms (ion-exchange, inner sphere complexation, physisorption, chemisorption, electrostatic, intercalation and other surface activation treatments). The overarching goal of this project is to develop new low-cost, efficient, and chemically/mechanically stable sorbent materials for off-gas radioiodine capture and immobilization based on MXenes of two-dimensional transition metal carbides/nitrides. The proposed exploratory research will focus on three main objectives: 1) design and synthesis of MXenes as radioiodine sorbent and support materials, 2) quantification of iodine sorption capacity of MXenes in different forms, and 3) synthesis and characterization of consolidated waste forms.