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Dear Editor,

On behalf of my co-authors and myself, I am hereby submitting our manuscript, entitled “*First-Principles Investigation of Lanthanides Diffusion in HCP Zirconium via Vacancy-Mediated Transport”* to the Journal of Nuclear Materials.

This article presents a density functional theory (DFT) study on the diffusion of lanthanide fission products in zirconium. The fuel-cladding chemical interaction (FCCI) in sodium-cooled fast reactors is a common cause of fuel pin failures. Introducing an interdiffusion barrier, such as a zirconium liner, between the fuel and cladding may mitigate the growth of the FCCI regions. However, the effectiveness of such liners in inhibiting the diffusion of lanthanide fission products has not been well investigated in the literature. In this article, we employed DFT and self-consistent mean field theory to calculate the exact transport coefficients of La, Ce, Pr, and Nd in hexagonal close-packed (HCP) Zr assuming a vacancy-mediated diffusion mechanism. La, Ce, and Pr behave as oversized solutes where they occupy an intermediate position between two half vacancies in the basal plane. To the best of our knowledge, the diffusion of oversized solutes in HCP crystal structures is unprecedented in the literature. The diffusivities of La, Ce, Pr, and Nd, and their segregation tendencies (enrichment or depletion at sinks) in HCP Zr are reported for the first time. The anisotropic diffusion and segregation tendencies of lanthanides in HCP Zr reported in this work present important insights about how to achieve better retention of lanthanides in Zr liners by controlling the grain texture during manufacturing. In addition, the calculated diffusion parameters in this study can serve as an input to fuel performance codes to quantitatively assess the effectiveness of Zr liners in mitigating FCCI.

Our study unveils novel insights into the diffusion behavior of lanthanide fission products within HCP Zr. We are confident that our findings hold significant value for the advancement of cladding liners tailored for metallic fuels in sodium-cooled fast reactors. Moreover, the analytical framework presented in our study holds considerable relevance for a wide spectrum of researchers within the scientific community who are engaged in the modeling of diffusion processes in metallic systems.

Sincerely,

Benjamin Beeler