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**Migration energies of native defects and fission products in uranium dioxide**[1] ALEXANDER THOMPSON, CHRIS WOLVERTON, Northwestern University — Despite the importance of fission products like Xe in nuclear fuels, the mechanism of how these atoms diffuse in the lattice is not known. In an effort to identify this mechanism, we have used density functional theory as well as a variety of different classical potentials for to study the migration energies of a variety of atomic steps in UO2, with and without Xe impurities and native defects. We find that the classical potential of Basak gives results which compare favorably with density functional theory for the diffusion of a Schottky defect cluster. We observe a new path for xenon-tetravacancy (a UO2 Schottky defect plus an additional U vacancy) motion using molecular dynamics. This path has a lower energy barrier than previously reported xenon-tetravacancy paths. We examine the possibility of a uranium vacancy dissociating from the xenon-tetravacancy cluster and find that large barriers for this dissociation. We also calculate xenon-double Schottky defect migration and find it has a slightly larger barrier than xenon-tetravacancy motion with the oxygen vacancies being weakly bound to the defect.

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