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Ab Initio Investigation of He Bubbles at the Y2Ti2O7-Fe Interface in Nanostructured Ferritic Alloys CELINE HIN, THOMAS DANIELSON, Virginia Tech — Nanostructured ferritic alloys are promising materials candidates for the next generation of nuclear reactors due to their ability to withstand high temperatures and pressures, high neutron flux and especially, the presence of high concentrations of transmutation product helium. As helium diffuses through the matrix, large number densities of complex oxide nanoclusters act as trapping sites for individual helium atoms and helium clusters. Consequently, there is a significant decrease in the amount of helium that reaches grain boundaries, mitigating the threat of pressurized bubble formation and embrittlement. In order to understand the trapping phenomena of the oxides, the interface between the nanoclusters and the iron matrix must be modeled. We present results obtained using density functional theory on the structural and thermodynamic properties of the Y2Ti2O7-Fe interface containing helium. In addition, helium bubbles of varying sizes have been introduced in order to observe the effects of a growing helium bubble

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