Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Energetics of Cs in 3 grain boundary of 3C-SiC[1] PUSHPA RAGHANI, Boise State University — Energetics of Cs defects at 3 grain boundaries of 3C-SiC has been studied using density functional theory to understand the role of the grain boundaries in Cs diffusion and its eventual release from the tristructural isotropic fuel particles (TRISO). Cs is shown to be much more stable at the 3 grain boundary than in bulk of SiC with a significant decrease (7 - 17 eV) in the formation energies at grain boundaries than in bulk. It is found to have even lower formation energies than those of Ag at the 3 grain boundaries, while this trend was opposite in the bulk SiC as demonstrated previously from similar density functional theory calculations. Based on these results, a possible route to control Cs release from SiC layer via grain-boundary-engineering is suggested.

[1]National Science Foundation

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Date submitted: 14 Nov 2013 Electronic form version 1.4