Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Interstitial and substitutional Zr in SrTiO3[1] JOHN JAFFE, RENEE VAN GINHOVEN, WEILIN JIANG, Pacific Northwest National Lab — We investigate Zr in $SrTiO_3$ (STO) as an electronic dopant and as a model for nuclear waste forms in which radioactive Sr decays to Y and then to stable Zr through beta emission. Density functional theory (DFT) within the supercell model is used to predict the thermodynamic stability and electronic states of interstitial and Sr- or Ti-substituted Zr atoms in the STO lattice. Native point defects such as vacancies and antisites are also considered. When Zr replaces Sr, its most stable configuration is to simply occupy the Sr site (instead of, for example, replacing a Ti and displacing the Ti to the Sr site.) For Zr added to the lattice, its most stable configuration is to replace a Ti, making a Zr_{Ti} impurity plus a Ti interstitial (as opposed to the Zr just remaining as an interstitial atom.) Zr_{Sr} is predicted to be a double electron donor, Zr_{Ti} is electrically inactive and interstitial Zr and Ti are predicted to be quadruple donors, with all donor levels in the conduction band. Zr_{Sr} and the tetravalent interstitials are all predicted to increase the crystal volume, and the interstitials also are predicted to lead to a tetragonal distortion of the lattice. Experiments with injection of Zr atoms into STO qualitatively confirm these predictions of crystal structural changes.

[1]Supported by U.S. Department of Energy Waste Form Campaign.

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Date submitted: 29 Dec 2010 Electronic form version 1.4