Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Theoretical Investigation of TI-Doped Zirconia Surfaces HASANI CHAUKE, Materials Modelling Centre, University of Limpopo, P/Bag x1106, Sovenga,0727, SA, RICARDO GRAU-CRESPO, Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, UK, PHUTI NGOEPE, Materials Modelling Centre, University of Limpopo, P/Bag x1106, Sovenga,0727, SA, NORA H. DE LEEUW, Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, UK — We use density functional theory calculations with Hubbard corrections (DFT+U) to investigate the electronic and redox properties of Ti-substituted zirconia (111) surfaces. It is found that titanium dopants are more likely to segregate at the surface than to migrate to the zirconia bulk. The formation energy of oxygen vacancies decreases substantially in titanium-substituted surfaces with respect to undoped surfaces. If an O vacancy is created around an isolated Ti dopant, a $Ti^{4+} \rightarrow Ti^{2+}$ reduction takes place, while if the vacancy is created in the vicinity of a pair of dopants, each Ti atom adopts a 3+ oxidation state, with additional decrease in the vacancy formation energy. We investigate in detail the relevant distribution of dopants and vacancies in the system, and discuss the implications of our results for some applications of zirconia-based ceramics.

Hasani Chauke
Materials Modelling Centre, University of Limpopo,
P/Bag x1106, Sovenga,0727, SA

Date submitted: 25 Nov 2009 Electronic form version 1.4