Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First principles studies of Ce and Eu-doped inorganic[1] ANDREW CANNING, ANURAG CHAUDHRY, ROSTYSLAV BOUTCHKO, STEPHEN DERENZO, Lawrence Berkeley National Laboratory — This work presents the results of first principles electronic structure calculations for europium and Ce doped inorganic compounds performed using the pseudopotential method based on the local spin density approximation (LSDA) and generalized gradient approximation+U (GGA+U) in density functional theory. The positions of the europium and cerium 4f and 5d states relative to the valence band maximum and conduction band minimum of the host material are determined. Qualitative predictions of the brightness of scintillation in the doped material is made based on the following criteria: (1) The size of the host material bandgap (2) The energy difference between the VBM (Valence Band Maximum) of the host material and the dopant 4f level (3) The energy difference between the occupied Eu or Ce 5d excited state and the host material CBM (Conduction Band Minimum) (4) The level of localization of the 5d excited state on the dopant atom. We have validated this theoretical approach on examples of known bright scintialltors and non-activated scintillators. We have performed calculations on new Eu doped compounds to determine if they are candidates for Eu2+ activated scintillators

[1]Research supported by the U.S. Department of Homeland Security

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Date submitted: 12 Dec 2008 Electronic form version 1.4