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**First Principles Calculations for Eu-doped Inorganic Scintillator Gamma Ray Detectors**[1] A. CANNING, Lawrence Berkeley National Lab, A. CHAUDHRY, UC Davis, R. BOUTCHKO, Lawrence Berkeley National Lab, N. GRONBECH-JENSEN, UC Davis, S.E. DERENZO, Lawrence Berkeley National Lab — This work presents the results of first principles electronic structure calculations for europium (Eu2+) 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 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 Eu2+ activated 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 Eu2+ 4f level (3) The energy difference between the occupied Eu 5d excited state (Eu2+)* and the host material CBM (Conduction Band Minimum) (4) The level of localization of the excited (Eu2+)* electron state on the Eu atom. We have validated this theoretical approach on examples of known bright scintillators like SrI2 and BaI2 and non-Eu activated scintillators. We have performed calculations on new Eu doped compounds to determine if they are candidates for Eu2+ activated scintillators.

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