Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-principles Investigation of the Structure, Mobility and Optical Properties of Self-Trapped Excitons in Alkali Metal, Lanthanum and Barium Halide Scintillators[1] GREGORY BIZARRI, MAURO DEL BEN, EDITH BOURRET, ANDREW CANNING, Lawrence Berkeley National Laboratory — The performance of new and improved materials for gamma ray scintillator detectors is dependant on multiple factors such as quantum efficiency, energy transport etc. In halide scintillator materials the energy transport is often impacted by self-trapped exciton (STE) formation and mobility. We present first-principles calculations at the hybrid density functional theory level for the structure, mobility and optical properties of STEs and their associated lattice defects (V_K centers) in two important families of scintillator materials, alkali metal and lanthanum halides (AX and LaX). AX and LaX have been extensively characterized by experiments and serve as benchmark systems to assess the accuracy of our theoretical procedure. We show that hydrid functionals accurately predict the different types of self-trapped excitons (on and off-center) found in AX and LX materials in agreement with EPR experiments. We then applied this approach to perform preliminary studies on classes of new scintillator materials including the barium mixed halides and compared with our new experimental results. These studies have the potential to benefit the development of improved scintillator materials tailored for specific applications.

[1]This work is supported by the U.S. Department of Energy/NNSA/DNN RD and is carried out at Lawrence Berkeley National Laboratory under Contract No. AC02-05CH11231

Andrew Canning
Lawrence Berkeley National Laboratory

Date submitted: 11 Nov 2016 Electronic form version 1.4