Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

A first-principles study of co-doping in lanthanum bromide[1]
DANIEL ABERG, BABAK SADIGH, Lawrence Livermore Natl Lab, ANDRE SCHLEIFE, University of Illinois at Urbana-Champaign, PAUL ERHART, Chalmers University of Technology — It was recently shown that the energy resolution of Ce-doped $LaBr_3$ scintillator radiation detectors can be crucially improved by co-doping with Sr, Ca, or Ba. Here we outline a mechanism for this enhancement on the basis of electronic structure calculations. We show that Sr dopants create and bind to Br vacancies, resulting in stable neutral complexes. The association with Sr causes the deep vacancy level to move toward the conduction band edge. This is essential for reducing the effective carrier density available for Auger quenching during thermalization of hot carriers. Subsequent de-trapping of electrons from the complexes can activate Ce dopants that have previously captured a hole leading to luminescence. This mechanism implies an overall reduction of Auger quenching of free carriers, which is expected to improve the linearity of the photon light yield with respect to the energy of incident electron or photon. Optical properties of the Ce-Sr-vacancy triple complex are discussed and compared to experiment. Prepared by LLNL under Contract DE-AC52-07NA27344.

[1]Support from the National Nuclear Security Administration Office of Nonproliferation Research and Development (NA-22) is acknowledged.

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Date submitted: 14 Nov 2014 Electronic form version 1.4