

Abstract Submitted
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First-principles Studies of the Role of Defects and Impurities on the Optical Properties of Barium Halide Storage Phosphors and Scintillator Materials¹ ANDREW CANNING, BHARAT MEDASANI, MAURO DEL BEN, EDITH BOURRET, GREGORY BIZARRI, Lawrence Berkeley National Laboratory — The Eu doped Ba mixed halide family BaBrX (X=F,Cl,Br,I) changes from being a widely used X-ray storage phosphor (BaBrF:Eu) to one of the brightest know new gamma ray detector scintillators (BaBrI:Eu). To help understand these contrasting optical properties and guide in the design of new and improved scintillator detectors, in collaboration with experimental groups, we have performed first principles theoretical studies of these materials. In particular we have studied their electron and hole trapping mechanisms associated with dopants, defects and impurities and how they can explain their very different optical properties.

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