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First-principles Studies of the Optical Properties of Eu doped Barium Halides: From Storage Phosphor to Bright Scintillator ANDREW CANNING, Lawrence Berkeley National Laboratory, UC Davis , BHARAT MEDASANI, MAURO DEL BEN, 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 and how that can explain their very different optical properties.

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