Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

**First-principles study of complex halide scintillators for radiation detection**[1] QINGGUO FENG, BYUNGKYUN KANG, JONATHAN MIZE, KOUSHIK BISWAS, Department of chemistry and physics, Arkansas State University, State University, Jonesboro, AR 72467, USA — Current demands for cost-effective and high-performance scintillators have led to a discernible shift from simple binary halides (e.g., NaI, CsI) toward host compounds that are structurally and electronically more complex. Eu-doped $SrI_2$ is a prominant example. Despite its advanced properties, improvements are needed for extensive deployment at low cost. Codoping techniques are often useful to improve the electronic response of such insulators. Using first-principles based approach we report on the influence of codoping with aliovalent and isovalent impurities. We find all codopants induce deep levels, show amphoteric character, and may bind with I-vacancy forming charge compensated donor-acceptor pairs. Lack of deep-to-shallow behavior upon codoping and its ramifications will be discussed. We studied another set of stable monoclinic phase of ternary $ns^2$ containing iodides, e.g. $TlBa_2I_5$. One objective is to explore them as scintillators where $ns^2$ ions play a central role. Interestingly, we predict $Eu^{2+}$ activation will be rendered ineffective in these compounds, caused by changes in the valence and conduction band edges. However, the prospect of fast electron capture at $ns^2$ sites and self-activated scintillation could be important for detector applications.

[1]This material is based upon work supported by the US Department of Homeland Security under Grant Award Number, 2014-DN-077-ARI075-04.

Qingguo Feng
Arkansas State University

Date submitted: 16 Nov 2016 Electronic form version 1.4