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Electronic Structure Engineering of Elpasolites for Brighter and Faster Scintillators MAO-HUA DU, Oak Ridge National Lab, KOUSHIK BISWAS, Department of Chemistry and Physics, Arkansas State University — Utilization of scintillator materials is one of the primary methods for radiation detection. Elpasolites are a large family of quaternary halides that have attracted considerable interest for their potential applications as γ-ray and neutron scintillators. However, many elpasolite scintillator materials currently under development suffer from low light yield and long scintillation decay time. The low light yield is partially due to a large band gap while the long scintillation decay time is a result of slow carrier transport to Ce dopants, where electrons and holes recombine to emit photons. We suggest that these problems may be mitigated by optimizing the band gap and carrier mobility by selecting constituent elements of proper electronegativity. For example, cations with lower electronegativity may lower the conduction band and increase the conduction band dispersion simultaneously, resulting in higher light yield and faster scintillation. First-principles calculations of electronic structure, small polarons, and Ce dopants in Cs_2LiYCl_6 and Cs_2AgYCl_6 compounds show that the strategy of manipulating electronegativity can lead to brighter and faster elpasolite-based scintillators. This work was supported by the U.S. DOE Office of Nonproliferation Research and Development NA22.

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