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Engineering Electronic Band Structure for New Elpasolite Scintillators MAO-HUA DU, KOUSHIK BISWAS, DAVID SINGH, Oak Ridge National Laboratory — The utilization of scintillator materials is one of the primary methods for radiation detection. Elpasolites are a large family of quaternary halides that have recently attracted considerable interest for their potential applications as γ-ray and neutron scintillators. A large number (on the order of 10^3) of different chemical compositions exist in the elpasolite family of compounds. This wide range of compositions offers numerous opportunities for fine-tuning the material chemistry to target specific scintillation properties, but they also pose significant challenges in identifying the most promising ones. Many elpasolite scintillator materials currently under development suffer from low light output and long scintillation decay time. The low light output is partially due to a large band gap while the long scintillation decay time is a result of the slow carrier transport to Ce impurities, where carriers 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 output and faster scintillation. We demonstrate by first-principles calculations that the strategy of manipulating electronegativity can lead to a number of new elpasolite compounds that are potentially brighter and faster scintillators.

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