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First-principles Electronic Structure Calculations for Scintillation Phosphor Nuclear Detector Materials[1]

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Inorganic scintillation phosphors (scintillators) are extensively employed as radiation detector materials in many fields of applied and fundamental research such as medical imaging, high energy physics, astrophysics, oil exploration and nuclear materials detection for homeland security and other applications. The ideal scintillator for gamma ray detection must have exceptional performance in terms of stopping power, luminosity, proportionality, speed, and cost. Recently, trivalent lanthanide dopants such as Ce and Eu have received greater attention for fast and bright scintillators as the optical 5d to 4f transition is relatively fast. However, crystal growth and production costs remain challenging for these new materials so there is still a need for new higher performing scintillators that meet the needs of the different application areas. First principles calculations can provide a useful insight into the chemical and electronic properties of such materials and hence can aid in the search for better new scintillators. In the past there has been little first-principles work done on scintillator materials in part because it means modeling f electrons in lanthanides as well as complex excited state and scattering processes. In this talk I will give an overview of the scintillation process and show how first-principles calculations can be applied to such systems to gain a better understanding of the physics involved. I will also present work on a high-throughput first principles approach to select new scintillator materials for fabrication as well as present more detailed calculations to study trapping process etc. that can limit their brightness. This work in collaboration with experimental groups has lead to the discovery of some new bright scintillators.

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