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First Principles Study of Phosphor Host Materials CLAIRE-ALICE HEBERT, Physics Department, University of California Santa Barbara, RAM SESHADRI, Materials Research Lab, University of California Santa Barbara — Solid state lighting uses light-emitting diodes (LEDs) instead of electrical filaments. Blue LEDs are combined with an inorganic phosphor consisting of a host lattice doped with Ce^{3+}. Electronic transitions between the 4f and 5d levels convert blue light from the diode to light ranging from green ($\sim$510 nm) to red ($\sim$700 nm) and the combination of yellow with blue creates white light. The most efficient phosphors have been found to have rigid crystal structures, along with band gaps large enough that the 4f to 5d transition of the dopant ion can occur without interference. Using Debye temperature as a proxy for structural rigidity, we use density functional theory (DFT) to calculate and plot Θ_D versus band gap to give us a prediction of phosphor suitability for forty different materials. PBE functionals and the quasi-harmonic Debye model were used to estimate Θ_D, and band gaps were calculated with a hybrid functional. DFT was also used to probe six potential hosts more closely: AlO_3, $LaBr_3$, Ba_2SiO_4, Sr_2SiO_4, $Sr_2Si_5N_8$, and $Y_3Al_5O_{12}$. The electronic states of these compounds were aligned with vacuum using a supercell slab model and will be compared with the Ce^{3+} levels to determine suitability as host materials.

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