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Electronic and Optical Properties of Luminescent Centers in Halides and Oxides

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Luminescent materials, such as phosphors and scintillators, are widely used for fluorescent lighting, laser, medical imaging, nuclear material detection, etc. . The luminescence is usually activated by impurities (or activators), which act as luminescence centers. The activators are typically multi-valent ions that insert multiple electronic states in the band gap of the host material. In this talk, first-principles calculations of electronic structure and optical transitions are shown for a wide range of activators, including rare-earth ions (e.g., Ce^{3+}, Eu^{2+}), ns^2 ions (the ions that have outer electronic configurations of ns^2, such as Tl^+, Pb^{2+}, Bi^{3+}), and transition-metal ions (e.g., Mn^{4+}), in a large number of halides and oxides. The results reveal how the activator-ligand hybridization affects the emission energy and the luminescence mechanism. New phosphors and scintillators are proposed based on the chemical trends emerging from the calculations of a large number of materials.