First-Principles investigation of the electronic structure of Phosphor materials doped with Transition Metal Ions

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Materials doped with transition metal ions (Mn^{4+}, Cr^{3+} and Ni^{2+}) recently have been extensively studied for application in the many fields such as w-LED, optical thermometry, bioimaging and others [1]. In this talk, we present the results of first-principles calculations on the Mn^{4+}, Cr^{3+} and Ni^{2+} doped phosphors materials. The purpose of our work is theoretical studies of the crystal and electronic structures of the ground and excited states and the optical transitions phosphors doped with these transition metal ions. Investigations based on first principles calculations were carried out in the framework of density functional theory (DFT) using the VASP code [2]. In the first step, the geometry of structure for the ground and excited states phosphors was optimized at GGA-PBE, GGA+U and SCAN levels. The calculation of optical transitions was performed on the basis of their optimized structures with different -GGA-PBE, GGA+U and HSE06 methods, respectively.

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