Electronic structure of Mn^{2+}-doped phosphors

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Nanocrystalline materials doped with transition metal ions (Mn^{4+}, Cr^{3+}, Mn^{2+}, Ni^{2+}) are promising materials due to their potential application in many fields. In particular, nanocrystalline materials doped with Mn^{2+} ions have become the object of intensive research due to their practical application as a source of NIR phosphors. In the present work we report on results of a density functional theory study of geometric and electronic structures and optical transition energy of Mn^{2+}-doped phosphors using various methods of calculations, in particular GGA-PBE, SCAN, HSEO6. The geometric and electronic structures and optical transitions of the Mn^{2+} ion being in tetrahedral and octahedral environments are analyzed following the technique [1,2]. As an example, Figure 1 presents the results of GGA-PBE calculations of DOS of Mn^{2+}-doped $KMgF_3$.

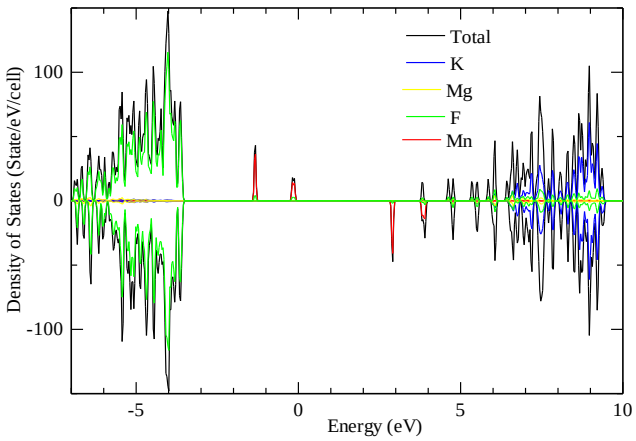

Figure 1. Density of states (DOS) of Mn^{2+} -doped $KMgF_3$.

[1] Umar Z., Khyzhun O., Yamamoto T., Brągiel P. (2024) Opt. Mater., 149, 115057.
[2] Umar Z., Kurboniyon M.S., et al. (2024) J. Lumin., 266, 120278.