# COMPARISON OF $Cs_2SiF_6$ AND $K_2SiF_6$ ADVANCED PHOSPHORS: FIRST PRINCIPLES CALCULATIONS

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The results of first-principles calculations of two advanced phosphors — cesium hexafluorosilicate ($Cs_2SiF_6$, CSF) and potassium hexafluorosilicate ($K_2SiF_6$, KSF), both defect-free and doped with Mn atoms — are discussed and compared. It is well known, that both compounds are suitable hosts for the study of the luminescence properties of different impurities in the octahedral crystal field [1–4].

The structural, electronic and elastic properties of perfect and doped materials are considered in detail. The simulations were performed using the CRYSTAL23 computer code [5] within the linear combination of atomic orbitals (LCAO) approximation of the density functional theory (DFT). To find an optimal combination of basis set and functional for the calculations, two basis sets and four different functionals (three advanced hybrid exchange-correlation and one LDA functionals) were used and compared with available experimental data. Further, for selected basis set and functional, the dependences of mentioned properties of pure CSF and KSF on pressure (0–20 GPa) were evaluated. In addition, the vibrational properties of pure materials were investigated and simulations of doped materials (CSF:$Mn^{4+}$ and KSF:$Mn^{4+}$) were performed. Impurities were considered using supercells containing 36 and 288 atoms. The local structural changes due to impurities and positions of defect levels in the band gap are studied in detail.

References

1. M.G. Brik, *Solid State Commun.*, 2010, 150, 1529–1533.

2. M.G. Brik, A.M. Srivastava, *J. Electrochem. Soc.*, 2012, 159, J212–J216.

3. M. Subhoni et al., *Opt. Mater.*, 2021, 115, 110986.

4. M.S. Kurboniyon et al., *J. Lumin.*, 2023, 263, 120103.

5. R. Dovesi et al., CRYSTAL23 User's Manual. University of Torino: Torino, 2022.