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Ab-initio study of the optical properties of Pr3+ doped fluoride crystals

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Abstract: The first-principle calculations are performed to study the optical properties of the rare earth Pr3+ doped fluoride crystals (MF2 ; M=Sr, Cd) using the full potential-linearized augmented plane wave method (FP-LAPW) [1] implemented in the code WIEN2K within the density functional theory (DFT) [2]. We present calculations based on Local Density Approximation LSDA and also on Coulomb-corrected LSDA+U [3, 4] approach because the rare earth compounds are highly correlated systems.
The ground-state properties have been calculated in the cubic structure. The optical properties such as the dielectric function, optical reflectivity, absorption coefficient, refractive index, extinction coefficient and electron energy loss are performed for the energy range of 0 - 40 eV.

References
[1] P. Blaha, K. Schwarz, P. Sorantin, S.B. Trickey, Comput. Phys. Commun. 59 (2), 399 (1990)
[2] P. Hohenberg, Phys. Rev. B36, 864 (1964),
[3] A.I. Liechtenstein, V.I. Anisimov and J. Zaanen, Density-functional theory and strong correlation: Orbital ordering in Mott-Hubbard insulators, Phys. Rev. B52, R5467 (1995)
[4] V.I. Anisimov, F. Aryasetiawan and A.I. Liechtenstein, First-principles calculations of the electronic structures and spectra of strongly correlated system: the LDA+U method, J. Phys. Condensed Matter, 9, 767, (1997)

Choix de session parallèle

5.3 SFO: Metamatériaux, plasmonique

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