The Improved Electronic Structure of the $LuVO_4$ Crystal Evaluated with the Strong Electron Correlation

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Due to exceptional optical properties, like wide optical transparency and large birefringence the zircon- and scheelite-type ABO4 compounds are potential candidates for optical isolators, circulators beam displacers and components for polarizing optics [1]. The zircon-type $LuVO_4$ crystal in tetragonal structure is described by space group 141 and its unit cell containes Z=4 formula units. The lutetium 4f- and vanadium 3d-electrons reveal the strong correlated behaviour, and therefore the LDA and GGA approaches in electronic structure are not adequate. So we employ the hybrid exchange-correlation functional similar to PBE0 [2] one:

$$E_{xc} = E_{xc}^{GGA} + a\,(E_x^{HF}(y_{4f}) - E_{xc}^{GGA}(r_{4f}) + E_x^{HF}(y_{4d}) - E_{xc}^{GGA}(r_{3d}))\,. \qquad (1)$$

The electronic structure (Fig. 1) has been evaluated by means of the ABINIT code.

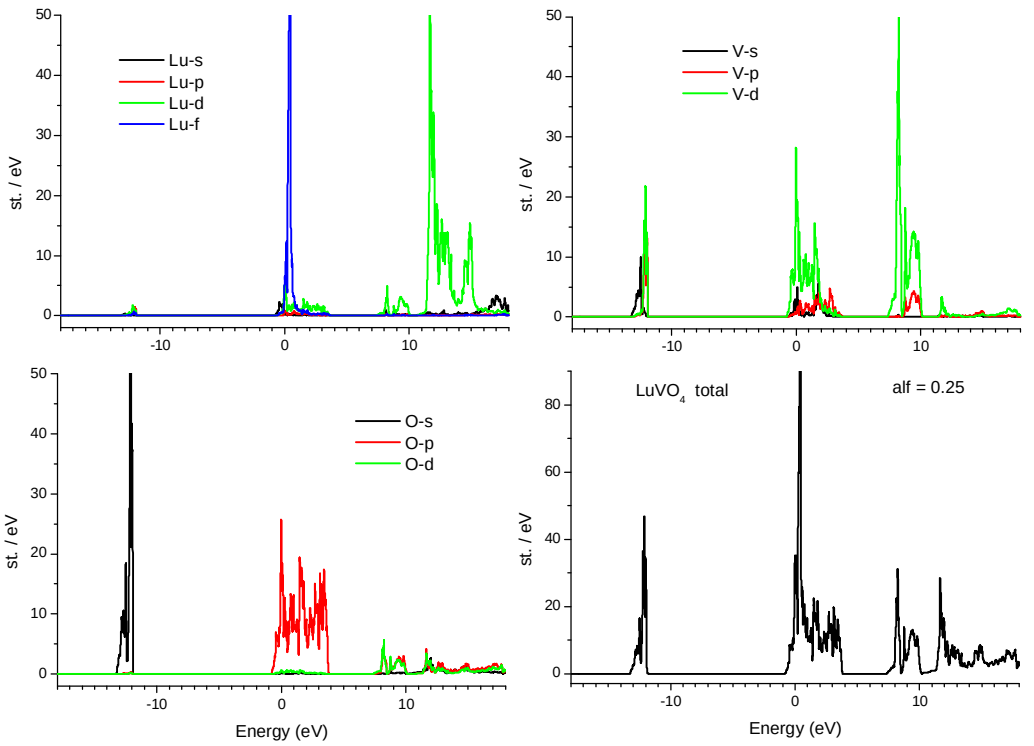

Figure 1. Partial and total DOS of the zircon $LuVO_4$ crystal found with a =0.25 value.

The obtained band gaps are: E_g = 3.05 eV (a =0), E_g = 3.46 eV (a =0.25) and E_g = 3.86 eV (a =0.45). Last calculated here value is well compared with experimental band gaps: 3.79 eV (reflectance), 3.76 eV (absorption) and 3.87 eV (emission).

[1] V. Panchal, D. Errandonea, A. Segura, P. Rodríguez-Hernandez, A. Muñoz, S. Lopez-Moreno, M. Bettinelli, *J. Appl. Phys.* **110** (2011) 043723.

[2] J. P. Perdew, M. Ernzerhof and K. Burke, *J. Chem. Phys.* **105** (1996) 9982.