Electronic and Magnetic Properties of $GdPO_4$ -*Ab-initio* Calculations

P. Leśniak,[1] W.L. Malinowski,[1] M. Werwiński,[1,2] A. Szczeszak,[3] T. Grzyb,[3] S. Lis,[3] B. Idzikowski,[1] and A. Szajek[1]

[1] *Inst. of Mol. Physics, PAS, Smoluchowskiego 17, 60-179 Poznań, Poland*

[2] *Dept. of Physics and Astronomy, Uppsala Univ., Uppsala, Sweden*

[3] *A. Mickiewicz University, Faculty of Chemistry, Department of Rare Earths, Umultowska 89b, 61-614 Poznań, Poland*

Among the multifunctional nanomaterials, those suitable for both optical and magnetic resonance imaging are of special interest (see [1] and the references therein). Rare earth (RE) orthophosphates crystallize in several crystal systems depending on the RE ion forming the compound as well as on synthesis conditions. $GdPO_4$ orders antiferromagnetically with T_N=0.77K [2]. To give insight into electronic and magnetic structures of the considered orthophosphate system we employed the full potential local orbital (FPLO [3]) method. We will present the band structure, local and total densities of electronic states as well as, after spin polarized calculations, the spin and orbital magnetic moments.

References:

[1] Sonia Rodriguez-Liviano et al., Inorg. Chem., **52** (2013) 647.

[2] M. Evangelisti et al., Phys. Rev. B **84** (2011) 094408.

[3] K. Köpernik, H. Eschrig, Phys. Rev. B **59** (1999) 1743.

Work supported by the National Science Centre grant: DEC-2011/01/B/ST3/02212