Hyperfine interactions in $Gd_2Ti_2O_7$ pyrochlore: *ab initio* calculations

Luciano Fabrício Dias Pereira[1], Wanderson Lobato Ferreira[1], Vítor Cavalcanti Gonçalves[1], Levy Scalise[1], Frederico Antônio Genezini[1], Eduardo Lima Corrêa[1], Rajendra Narain Saxena[1] and Artur Wilson Carbonari[1]

[1] *Instituto de Pesquisas Energéticas e Nucleares, Universidade de São Paulo, São Paulo, Brazil.*

E-mail: lpereira@ipen.br

The cubic pyrochlore structure of the $RE_2Ti_2O_7$ (R= rare earth) form is highly geometrically frustrated antiferromagnets and $Gd_2Ti_2O_7$ is particularly interesting due to the fact gadolinium has a large magnetic moment and its orbital momentum is zero. Up to nowadays, a few investigations of the local structure on $Gd_2Ti_2O_7$ using hyperfine interactions techniques were made. Namely, the magnetic hyperfine interaction at Gd previously reported from Mossbauer effect spectroscopy with ^{155}Gd [1] and perturbed angular correlation (PAC) have used to reach electric field gradient at ^{111m}Cd and ^{111}In probe nuclei [2]. However, these studies are lacking in interpretation, so first principles calculations may *led to the elucidation of the electronic structure at the specific crystalline site. Then,* $Gd_2Ti_2O_7$ single and doped-Cd cell simulations have performed with full potential linearized augmented plane waves methods and generalized gradient approximation from Perdew-Burke-Ernzerhorf within the WIEN2k code. Electric field gradient and magnetic hyperfine components were evaluated.

[1] P. Bonville, J. A. Hodges, M. Ocio, *et al., J. Phys.: Condens. Matter*, **2003**, *Vol 15*, p. 7777–7787.

[2] E. L. Corrêa, A. W. Carbonari, L. F. D. Pereira, *et al.,* to be published.

[3] P. Blaha, K. Schwarz, G. K. H. Madsen, *et al.,* WIEN2k, **2001**, Vienna University of Technology, Austria.