Hyperfine interactions in Gd$_2$Ti$_2$O$_7$ pyrochlore: \textit{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.

\textit{E-mail: lpereira@ipen.br}

The cubic pyrochlore structure of the \textit{RE}_2\textit{Ti}_2\textit{O}_7 \ (\textit{R}= \text{rare earth}) form is highly geometrically frustrated antiferromagnets and Gd$_2$Ti$_2$O$_7$ 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$_2$Ti$_2$O$_7$ 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 \textit{led to the elucidation of the electronic structure at the specific crystalline site. Then, Gd}_2\textit{Ti}_2\textit{O}_7 single and doped-Cd cell simulations have performed with full potential linearized augmented plane waves methods and generalized gradient approximation from Perdew-Burke-Ernzerhof within the WIEN2k code. Electric field gradient and magnetic hyperfine components were evaluated.}

