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Lattice site and excited electronic states of implanted rare earth 172Lu ions in Ga2O3

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Gallium oxide (Ga2O3) belongs to the family of transparent conductive oxides, electrically conductive materials that are optically transparent. These materials have been widely studied due to their technological applicability, and Ga2O3, having the widest band-gap among them (4.8 eV), is a very interesting material for photonic applications working in the visible and UV wavelength region.
These functionalities might be enhanced by doping Ga2O3 with optically active rare earth (RE) ions due to their sharp and mostly temperature stable RE emission lines, whose spectral range spans from the infrared to the ultraviolet.
In this context, Perturbed Angular Correlation (PAC) measurements were performed after implantation of RE 172Lu probes into Ga2O3 polycrystalline samples in order to study the lattice site of the implanted RE ions. Moreover, because 172Lu decays by electron capture, it was possible to study the recombination of ionized and excited electronic states of the impurity/dopant as a function of temperature.
These results were later compared to Density Functional Theory (DFT) simulations via the implementation of different atomic local models, where the electric field gradient of each configuration was calculated.

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