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Electronic and structural properties of the α -Fe₂O₃:Ta semiconductor. Experimental EFG determination and ab initio calculations.

In this work we present results from Time-Differential Perturbed-Angular Correlations (PAC) experiments in α -Fe₂O₃ singlecrystals (in their corundum structure) implanted with ¹⁸¹Hf(\rightarrow ¹⁸¹Ta) ions at the ion accelerator facility of the H-ISKP at the Bonn University. The magnitude, asymmetry and orientation of the EFG were determined measuring the spin-rotation curves as a function of the singlecrystal orientation (for three different configurations of the sample) with respect to the laboratory system. The PAC experiments were carried out at 973 K in order to have only the electric-quadrupole interaction in the spectra, since above the Neel temperature (TN=955 K) the system has a paramagnetic behaviour.

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