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First-principles calculations and perturbed angular correlation experiments in BaMnO3 and MnAs

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We report on perturbed angular correlation (PAC) spectroscopy studies on magnetic compounds BaMnO3 and MnAs. Hyperfine parameters, e.g., the local Electric Field Gradient and Hyperfine Magnetic Field were measured by using the isotope probes 111Cd in BaMnO3 and 77Se in MnAs. MnAs was measured in a short range of temperatures near the first order magneto-structural transition at T=45 C. For the case of BaMnO3 we present results in the hexagonal 6-layered phase, from liquid nitrogen temperature until 700 C.
To model the hyperfine parameters obtained in the PAC experiments we are using the FP-APW+lo (full potential - augmented plane waves + local orbitals) method of density functional theory, as implemented in the Wien2k code [1]. The simulations consider the use of supercells that characterize different lattice sites and local configurations of the probe atoms, with increasing dilution to account for the ppm concentration range of the radioactive probes used in the experiments.
On these preliminary experimental-theoretical combined studies we provide now the information of the probe site, interpret the structural charge and magnetic local properties around the probe and prepare more detailed studies of the materials behavior upon temperature changes.

References:
[1] Peter Blaha, Karlheinz Schwarz, Georg K. H. Madsen, Dieter Kvasnicka, Joachiim Luitz: WIEN2k - An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties, Techn. Universität Wien Getreidemarkt 9/156 A-1060 Wien/Austria, ISBN 3-9501031-1-2.

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