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Insights into the magnetic ground state of Fe_2P from μSR, NMR and DFT perspectives

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Fe_2P alloys have been proposed as promising for applications in magnetocaloric refrigeration due to their first-order magnetic transitions coupled to a magnetoelastic transition, which gives rise to a giant magnetocaloric effect in the vicinity of their Curie temperature [1]. The magnetic structure of Fe_2P has been investigated and known to order ferromagnetically, with magnetic moments along the c-axis. However, these earlier sparse and often very old literature on Fe_2P are characterized by inconsistencies in the quantitative description of the Fe_1 magnetic moment size and the presence of helical states below T_c.

Here, using a combined effort of two spectroscopic techniques, μSR and NMR, in addition to DFT calculations, we have accurately characterized the magnetic ground state of Fe_2P. We perform zero applied field measurements using both experimental techniques below the ferromagnetic transition T_C = 220 K [2]. Our DFT calculations reproduce the experimental results and further allow us to improve their interpretation. We show a detailed characterization of the microscopic coupling between the electrons and P-nuclei or the muon in Fe_2P, which where then utilized to discuss the microscopic origin of the NMR and μSR resonances. Particularly, the computational predictions allow to identify correctly a previously mis-attributed signal from ^{31}P nuclei, an information relevant for future experiments. This work completely characterizes the signal of two technique of election for the characterization of magnetic properties, thus providing an important base for further analysis of different alloy compositions.

References

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Primary authors: Dr ONUORAH, Ifeanyi John (Department of Mathematical, Physical and Computer Sciences, University of Parma, 43124 Parma, Italy); Dr BONFÀ, Pietro (Department of Mathematical, Physical and Computer Sciences, University of Parma, 43124 Parma, Italy)

Co-authors: Dr ISAH, Muhammad Maikudi (Department of Mathematical, Physical and Computer Sciences, University of Parma, 43124 Parma, Italy); FRANDSEN, Benjamin (Brigham Young University); GIBSON, Ethan J. (Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA); BRÜCK, Ekkes (Fundamental Aspects of Materials and Energy (FAME), Faculty of Applied Sciences, Delft University of Technology, 2629 JB Delft, The Netherlands); Prof. DE RENZI, Roberto (Department of Mathematical, Physical and Computer Sciences, University of Parma, 43124 Parma, Italy); Prof. ALLODI, Giuseppe (Department of Mathematical, Physical and Computer Sciences, University of Parma, 43124 Parma, Italy)

Presenter: Dr ONUORAH, Ifeanyi John (Department of Mathematical, Physical and Computer Sciences, University of Parma, 43124 Parma, Italy)

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