

New insights into the complex magnetic behaviour of Mn_5Si_3

<u>Nikolaos Biniskos</u>¹, Flaviano José dos Santos², Karin Schmalzl³, Stéphane Raymond⁴, Manuel dos Santos Dias⁵, Stefan Blügel⁵, Samir Lounis⁵, Thomas Brückel⁶

¹Forschungszentrum Jülich GmbH (Jülich Centre for Neutron Science at MLZ, Lichtenbergstrasse 1, 85748 Garching, Germany), ²École Polytechnique Fédérale de Lausanne (Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), 1015 Lausanne, Switzerland), ³Forschungszentrum Jülich GmbH (Jülich Centre for Neutron Science at ILL, 38000 Grenoble, France), ⁴CEA-Grenoble (Université Grenoble Alpes, CEA, IRIG, MEM, MDN, 38000 Grenoble, France), ⁵Forschungszentrum Jülich GmbH (Peter Grünberg Institut & Institute for Advanced Simulations, 52425 Jülich, Germany), ⁶Forschungszentrum Jülich GmbH (Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, 52425 Jülich, Germany)

e-mail: n.biniskos@fz-juelich.de

The anomalous Hall effect (AHE) in ferromagnets manifests as a transverse voltage drop to the applied current in zero external magnetic field, and it is usually proportional to the magnetization. The AHE is often believed to be negligible in antiferromagnets (AFM) due to their vanishing net magnetization. However, recent studies have demonstrated that certain noncollinear AFM exhibit a large AHE that can be potentially exploited for future spintronic devices [1-2].

In this context Mn_5Si_3 is a promising material for applications since interesting transport and thermodynamic phenomena occur, such as the AHE [3] and the inverse magnetocaloric (MCE) [4]. Mn_5Si_3 undergoes two phase transitions towards a collinear and non collinear AFM phase at T_{N2} =100K (AFM2) and T_{N1} =66K (AFM1), respectively. The noncollinear spin configuration of this system, which is believed to be the origin of its important properties, is up to debate as different neutron diffraction studies proposed different magnetic structures [5-6]. In this work, we investigate Mn_5Si_3 using unpolarized and polarized inelastic neutron scattering (INS) measurements and density functional theory calculations [7-8]. We report the main magnetic exchange couplings for both AFM phases. Furthermore, we compute the spin-wave dispersions and compare them with the INS data. Finally, we investigate the effect of an applied magnetic field upon the magnetic structure and propose a model for the stability of some of the materials Mn moments.

[1] S. Nakatsuji et al, Nature 527, 212 (2015). [2] N. Kiyohara et al, Phys. Rev. Applied 5,

064009 (2016). [3] C. Sürgers et al, Scientific Reports 7, 42982 (2017). [4] N. Biniskos et al; Physical Review Letters 120, 257205 (2018). [5] P. J. Brown et al, Journal of Physics: Condensed Matter 4, 10025 (1992). [6] M. Gottschilch et al, Journal of Materials Chemistry 22, 15275 (2012). [7] F.J. dos Santos et al; Phys. Rev. B 103, 024407 (2021). [8] N. Biniskos et al; arXiv:2112.03368