Strong Correlation Effects in the Magnetic Kagome Materials Fe_3Sn and Fe_3Sn_2

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Abstract. Kagome materials have recently attracted significant attention due to their unique geometry, which promotes the formation of flat bands, topological features, and complex magnetic structures. Among these materials, Fe-Sn binary compounds have been particularly well studied, owing to the presence of various metastable phases with different stoichiometries that allow for control over the system dimensionality [1]. Understanding the interplay between magnetism and electronic structure in Fe-Sn binaries is therefore highly relevant for technological applications, as it may enable the exploitation of these systems in electronics and spintronics. In this study, we investigate the electronic and magnetic properties of Fe_3Sn and Fe_3Sn_2 by means of a combination of density-functional theory (DFT) and dynamical mean-field theory (DMFT), as implemented in the all-electron code RSPt [2]. We perform a detailed analysis of the magnetic anisotropy and exchange coupling, revealing the critical role of strong electronic correlations. Flat bands and topological features are shown to undergo substantial renormalization in DFT+DMFT calculations, suggesting that they may lie much closer to the Fermi energy than previously hypothesized [3]. This implies that they could be more easily manipulated through external stimuli such as doping or epitaxial strain. A detailed understanding of the electronic structure is essential for identifying signatures of topological states in experimental data, such as those obtained from angle-resolved photoemission spectroscopy (ARPES) [4]. Finally, we also investigate the anisotropic exchange coupling, including the Dzyaloshinskii–Moriya interaction. Although these contributions are significant in absolute terms, they are much smaller than the isotropic exchange, indicating the likely absence of magnetic chirality, at least at ambient conditions.

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