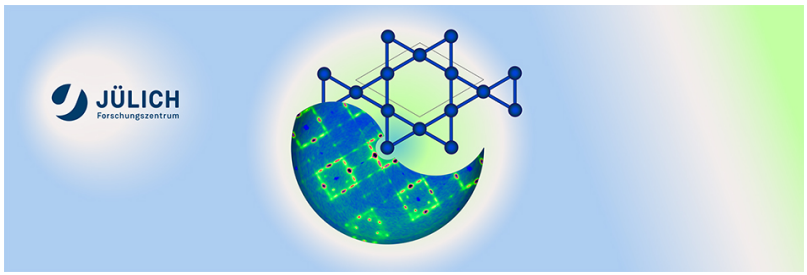

Beitrag ID: **109** Typ: **Invited talk**

Multiscale Modeling of Magnetic Ordering in Weyl Semimetals

Donnerstag, 9. Oktober 2025 09:00 (30 Minuten)

Magnetic Weyl semimetals are fascinating topological materials that exhibit complex magnetic orders. Here I focus on rare-earth and transition-metal-based magnetic Weyl semimetals. Rare-earth (RE) compounds such as REAlSi are examined using first-principles simulations to explore the connection between helical magnetic ordering and the emergence of Weyl nodes in electronic band structure [1]. The ab-initio based atomistic spin dynamics analysis reveals that the helical ordering is neither driven by Fermi-surface nesting nor by the Dzyaloshinskii–Moriya interaction; instead, it arises from frustrated, isotropic short-range superexchange interactions in the presence of crystal-field effects on the RE-sites [2]. Building on this, I discuss TM3X Kagome magnet family (TM = Mn, Fe; X = Ga, Ge, Sn), some of which are identified as magnetic Weyl semimetals, and introduce a novel computational approach for modeling complex non-collinear magnetic orders relying on the cluster multipole (CMP) method [3] in conjunction with atomistic spin Hamiltonians [4]. The magnetic ground state of the TM3X compounds is accurately reproduced by comparing the energies of candidate CMP configurations within a spin Hamiltonian that includes isotropic exchange, relativistic anisotropic terms, and higher-order biquadratic interactions [4]. The evaluation of CMP configuration energies at the model level is computationally efficient and enables high-throughput screening of complex magnetic ordering across a wide variety of materials.

[1] J. Gaudet et al. Nature Materials 20, 1650–1656 (2021).
[2] J. Bouaziz et al. Phys. Rev. B 109, L201108 (2024).
[3] M. T. Suzuki et al., Phys. Rev. B 95, 094406 (2017).
[4] J. Bouaziz et al. Phys. Rev. B 112, 014406 (2025)

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Sitzung Einordnung: Models of quantum magnetic systems