

Sunny.jl: A Julia Package for Spin Dynamics

David Dahlbom ^{1,2}, Hao Zhang ³, Cole Miles ⁴, Sam Quinn ^{5,6}, Alin Niraula ⁷, Bhushan Thipe ⁷, Matthew Wilson ⁸, Sakib Matin ³, Het Mankad ⁹, Steven Hahn ⁹, Daniel Pajerowski ¹, Steve Johnston ^{2,10}, Zhentao Wang ¹¹, Harry Lane ^{12,13,14}, Ying Wai Li ¹⁵, Xiaojian Bai ⁷, Martin Mourigal ⁵, Cristian D. Batista ², and Kipton Barros ³

1 Neutron Scattering Division, Oak Ridge National Laboratory, United States of America **2** Department of Physics and Astronomy, University of Tennessee, United States of America **3** Theoretical Division and CNLS, Los Alamos National Laboratory, United States of America **4** Kodiak Robotics, United States of America **5** School of Physics, Georgia Institute of Technology, United States of America **6** Department of Physics and Astronomy, University of California, Los Angeles, United States of America **7** Department of Physics and Astronomy, Louisiana State University, United States of America **8** X-Computational Physics Division, Los Alamos National Laboratory, United States of America **9** Computer Science and Mathematics Division, Oak Ridge National Laboratory, United States of America **10** Institute for Advanced Materials and Manufacturing, University of Tennessee, United States of America **11** Center for Correlated Matter and School of Physics, Zhejiang University, People's Republic of China **12** Department of Physics and Astronomy, University of Manchester, United Kingdom **13** The University of Manchester at Harwell, University of Manchester, United Kingdom **14** School of Physics and Astronomy, University of St Andrews, United Kingdom **15** Computer, Computational, and Statistical Sciences Division, Los Alamos National Laboratory, United States of America  Corresponding author

DOI: [10.21105/joss.08138](https://doi.org/10.21105/joss.08138)

Software

- [Review](#) 
- [Repository](#) 
- [Archive](#) 

Editor: [Sophie Beck](#) 

Reviewers:

- [@jabirali](#)
- [@Chronum94](#)

Submitted: 23 December 2024

Published: 20 December 2025

License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](https://creativecommons.org/licenses/by/4.0/)).

Summary

Sunny is a Julia package designed to serve the needs of the quantum magnetism community. It supports the specification of a very broad class of spin models and a diverse suite of numerical solvers. These include powerful methods for simulating spin dynamics both in and out of equilibrium. Uniquely, it features a broad generalization of classical and semiclassical approaches to $SU(N)$ coherent states, which is useful for studying systems exhibiting strong spin-orbit coupling or local entanglement effects. Sunny also offers a well-developed framework for calculating the dynamical spin structure factor, enabling direct comparison with scattering experiments. Ease of use is a priority, with tools for symmetry-guided modeling and interactive visualization.

Statement of need

Progress in quantum magnetism depends on the development of accurate models of magnetic materials. Scattering techniques, such as inelastic neutron scattering (INS) and resonant inelastic X-ray scattering (RIXS), are among the most informative methods available for probing the dynamics of quantum magnets, yielding the dynamical spin structure factor $\mathcal{S}(\mathbf{q}, \omega)$ as experimental output. To evaluate the validity of a hypothetical model, it is necessary to calculate $\mathcal{S}(\mathbf{q}, \omega)$ theoretically. This is generally an intractable problem that must be treated numerically or with various approximation schemes. The difficulty of this step represents a bottleneck in the development of accurate models and impedes the advancement of our understanding of quantum materials.

The Sunny project is a collaborative effort among theorists, experimentalists and computational scientists aimed at developing theoretical and numerical methodologies for modeling realistic quantum magnets. The central product of this effort is the Sunny software package, which

makes recent theoretical advances available in a form readily accessible to students and researchers. Distinguishing features of Sunny include:

- Symmetry analysis tools that facilitate model specification, visualization and data retrieval.
- A suite of optimizers, Monte Carlo samplers, and spin dynamics solvers that can all be applied to the same system specification.
- Implementation of the $SU(N)$ coherent state formalism for classical and semiclassical calculations.
- An interface tailored toward the needs of scattering scientists, with tools for integrating scattering intensities over regions of reciprocal space.
- Code written entirely in Julia, a language that can achieve speeds comparable to C++ or Fortran while offering an interactive workflow that will be familiar to users of Python and Matlab.
- A well documented codebase, an extensive collection of correctness tests, a website featuring many tutorials, and an active Slack channel where users can ask questions.

There are a number of existing codes that can calculate $\mathcal{S}(\mathbf{q}, \omega)$ using linear spin wave theory (LSWT), some of which have served as inspiration to the Sunny project (Hahn et al., 2024; Li, 2024; Petit & Damay, 2016; Rotter, 2004; Weber et al., 2016). The symmetry analysis tools of SpinW in particular have served as a model (Toth & Lake, 2015). There are also codes that perform classical spin simulations using Landau-Lifshitz (LL) dynamics (Bergman et al., 2024; Evans et al., 2014; Müller et al., 2019). Sunny is unique in offering both approaches and generalizing them through a formalism based on $SU(N)$ coherent states (Muniz et al., 2014; Zhang & Batista, 2021). Sunny additionally permits completely general single-ion anisotropies and coupling of multipolar moments, provides an efficient implementation of long-range dipole-dipole interactions, automates the application of a number of quantum renormalizations (Dahlbom et al., 2025), and offers iterative solvers for efficient LSWT on large magnetic cells (Lane et al., 2024).

The value of collecting all these tools together in a modern, easy-to-use package is evidenced by the large number of publications that have already made use of Sunny, a partial list of which is maintained on the GitHub wiki (Barros et al., 2025). We note a number of experimental studies that have relied on Sunny for analysis (Bai et al., 2021, 2023; Do et al., 2023; Kim et al., 2023; Lee et al., 2023; Na et al., 2024; Nagl et al., 2024; Paddison et al., 2024; P. Park et al., 2023; P. Park, Sala, et al., 2024; P. Park, Ghioldi, et al., 2024; Pyeongjae Park et al., 2025; Scheie et al., 2023), as well as theoretical and methodological works (Dahlbom, Brooks, et al., 2024; Dahlbom, Thomas, et al., 2024; Zhang et al., 2023; Zhang & Lin, 2024). Additional papers documenting the theoretical and algorithmic advances that have enabled the development of Sunny are discussed below.

Feature Overview

Symmetry analysis

By unifying and extending existing open source frameworks for the symmetry analysis of crystals – including Spglib (Togo et al., 2024), Brillouin.jl (Christensen et al., 2024), and CrystalInfoFramework.jl (Hester & Richard, 2024) – Sunny facilitates the process of determining the complete set of interactions allowed by spacegroup symmetries. Similarly, any interaction specified on a site or bond will be automatically propagated to all symmetry-equivalent sites and bonds, as required by the spacegroup symmetries. Models may also be specified according to symmetry properties and subsequently made “inhomogenous,” allowing the arbitrary modification of pair interactions and site properties without regard to symmetry constraints. This greatly facilitates the modeling of systems exhibiting chemical disorder. Finally, the symmetry information enables convenient specification of paths and slices through reciprocal space, aiding visualization and comparison to experimental data. All these tools can be applied

just as easily to a user-specified crystal or to a crystal loaded from an industry-standard CIF file (Hall et al., 1991).

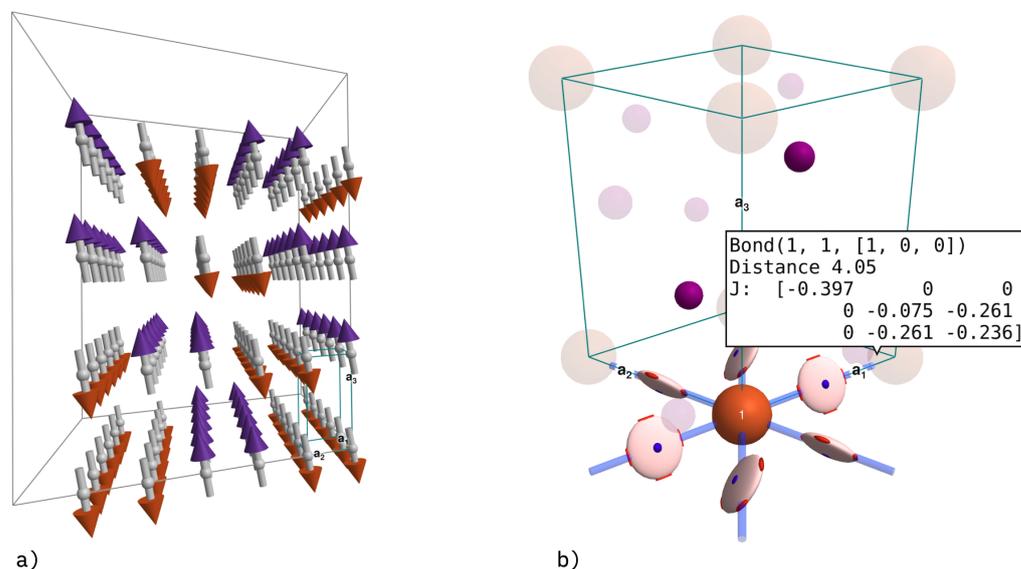


Figure 1: a) Ground state of FeI₂, found using Sunny's minimize_energy! function and visualized with plot_spins. b) The crystal of FeI₂ visualized with the view_crystal function. Hovering the cursor over a bond reveals the exchange interaction, if already assigned, or a general expression for all symmetry-allowed interactions.

Visualization

Both the symmetry analysis and data retrieval features of Sunny include 3D visualization tools built on the Makie package (Danisch & Krumbiegel, 2021). These can be used to plot spin configurations, investigate the symmetries of a crystal (Figure 1), generate animations of dynamic behavior, and plot the predicted results of scattering experiments (Figure 2).

SU(*N*) Formalism and System Modes

Traditional classical and semiclassical approaches to spin dynamics are based on the assignment of a classical dipole to each lattice site. Recent theoretical work has generalized this picture, replacing dipoles with richer objects, namely SU(*N*) coherent states. Such states capture the full structure of an *N*-level quantum system. Setting $N = 2s + 1$ enables the faithful representation of a quantum spin *s* and of the crystal field levels of a single-ion. The formalism can also be adapted to model local entanglement effects, where this entanglement may be between the spin and orbital degrees of freedom on a single site or within a cluster of spins on different sites.

The SU(*N*) formalism applies equally to LSWT calculations (Muniz et al., 2014) and classical spin dynamics (Zhang & Batista, 2021). Users can access this framework simply by setting the “mode” of a spin system to :SUN. Sunny also offers a :dipole mode, which is similar to the traditional classical approach but includes quantum renormalizations of biquadratic and single-ion anisotropy terms (Dahlbom et al., 2025). Finally, there is a mode that implements the traditional approach without any additional corrections, :dipole_uncorrected. Most Sunny features are supported in all modes.

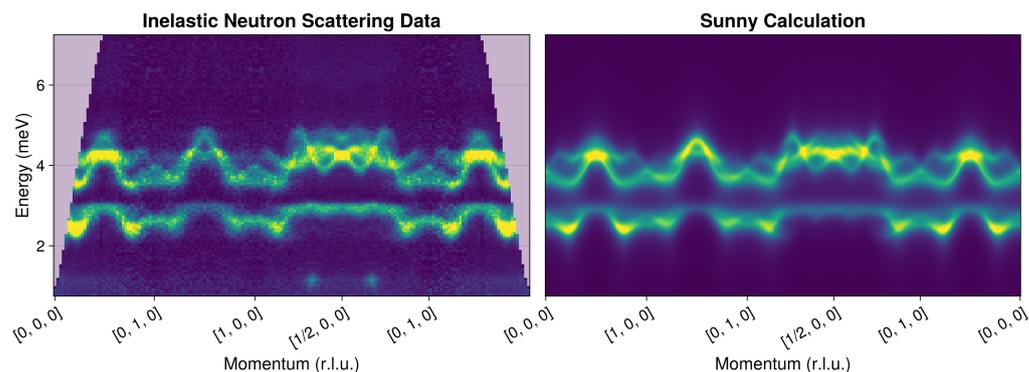


Figure 2: *Left:* Scattering intensities of FeI_2 as measured on the SEQUOIA instrument at the Spallation Neutron Source, Oak Ridge National Laboratory (Bai et al., 2021). *Right:* Predicted scattering intensities calculated with Sunny's $\text{SU}(N)$ linear spin wave solver. The figure was generated with Sunny's data retrieval and plotting functions.

Optimization and Monte Carlo Tools

Identifying a classical ground state is often the first step when calculating the scattering response of a magnet. Sunny provides several tools for finding such states, including gradient optimizers built on the Optim.jl package (Mogensen & Riseth, 2018). These optimizers work on supercells as well as spiral orderings. Sophisticated Monte Carlo tools are also provided, which can be used both to anneal into ground states and to estimate finite temperature statistics. In particular, the classical dynamics can be run with Langevin coupling to a thermal bath (Dahlbom, Miles, et al., 2022), and samplers are provided that implement the Wang-Landau (Wang & Landau, 2001) and parallel tempering algorithms (Swendsen & Wang, 1986).

Linear Spin Wave Theory (LSWT)

Sunny has extensive support for LSWT calculations, including for systems with arbitrarily complex single-ion anisotropies, general bilinear and biquadratic interactions, and long-range dipole-dipole interactions. Like SpinW, Sunny provides efficient LSWT calculations for systems that exhibit incommensurate spiral orderings (Toth & Lake, 2015). Additionally, Sunny provides tools to efficiently calculate $\mathcal{S}(\mathbf{q}, \omega)$ on very large magnetic cells using iterative matrix-vector multiplications (Lane et al., 2024). The simulation of large supercells is essential to study systems with chemical disorder or complex magnetic orderings.

Classical Dynamics

The efficiency of LSWT calculations makes it the preferred tool when studying magnets near zero temperature. At elevated temperatures or in out-of-equilibrium conditions, however, classical dynamics becomes a valuable technique. Sunny supports both traditional Landau-Lifshitz dynamics and its generalization to $\text{SU}(N)$ coherent states (Zhang & Batista, 2021). Dissipationless trajectories are calculated using a symplectic integration scheme (Dahlbom, Zhang, et al., 2022), and a generalization of the stochastic Landau-Lifshitz-Gilbert equations to $\text{SU}(N)$ coherent states (Dahlbom, Miles, et al., 2022) enables the simulation of dynamics coupled to a thermal bath. This is particularly valuable for simulating, e.g., thermal transport, pump-probe experiments, and spin-glass relaxation.

Sunny as a Platform for Future Developments

To make these existing features more widely available, work at Oak Ridge National Laboratory is underway to integrate Sunny into the Calvera platform for neutron data analysis (Watson

et al., 2022). Sunny itself can serve as a platform for new solvers and analysis techniques, building on its mature model specification and data retrieval features. Current efforts are directed at supporting: the self-consistent Gaussian approximation for diffuse scattering, enabling functionality inspired by (Paddison, 2023); the modeling of local entanglement effects generated by spin-orbit coupling or strongly coupled clusters of spins; non-perturbative corrections to LSWT for the modeling of continua and bound states, which can be probed in INS and terahertz spectroscopy experiments (Bai et al., 2023; Legros et al., 2021); and observables relevant to RIXS experiments.

Acknowledgements

We thank Mosé Giordano and Simon Danisch for valuable discussions. This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award Numbers DE-SC0022311, DE-SC-0018660, and DE-SC0025426. The work was also sponsored by the Laboratory Directed Research and Development Programs (LDRD) at Los Alamos National Laboratory, managed by Triad National Security, LLC, and at Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy. Applications to inverse scattering were partially supported by the National Science Foundation Materials Research Science and Engineering Center program through the UT Knoxville Center for Advanced Materials and Manufacturing (DMR-2309083). Z.W. acknowledges support from the National Key Research and Development Program of China (Grant No. 2024YFA1408303) and the National Natural Science Foundation of China (Grant No. 12374124). H.L. acknowledges funding from the Royal Commission for the Exhibition of 1851. The data shown in Figure 2 was collected at the the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory. Beam time was allocated to the SEQUOIA instrument on proposal number IPTS-21166.

References

- Bai, X., Zhang, S.-S., Dun, Z., Zhang, H., Huang, Q., Zhou, H., Stone, M. B., Kolesnikov, A. I., Ye, F., Batista, C. D., & others. (2021). Hybridized quadrupolar excitations in the spin-anisotropic frustrated magnet FeI_2 . *Nature Physics*, 17(4), 467–472. <https://doi.org/10.1038/s41567-020-01110-1>
- Bai, X., Zhang, S.-S., Zhang, H., Dun, Z., Phelan, W. A., Garlea, V. O., Mourigal, M., & Batista, C. D. (2023). Instabilities of heavy magnons in an anisotropic magnet. *Nature Communications*, 14(1), 4199. <https://doi.org/10.1038/s41467-023-39940-1>
- Barros, K., Dahlbom, D. A., Miles, C., Quinn, S., Zhang, H., Wilson, M., Thipe, B., Lane, H., Niraula, A., Bai, X., Matin, S., Giordano, M., Hahn, S., & others. (2025). Sunny.jl. In *GitHub repository*. GitHub. <https://doi.org/10.5281/zenodo.11363938>
- Bergman, A., Hellsvik, J., Rieger, P., Salehi, N., Chico, J., Priessnitz, J., & others. (2024). UppASD. In *GitHub*. GitHub. <https://github.com/UppASD/UppASD>
- Christensen, T., Barros, K., Herbst, M. F., Kim, S., Lihm, J. M., Holy, T., & Zhang, Q. (2024). Brillouin.jl. In *GitHub repository*. GitHub. <https://github.com/thchr/Brillouin.jl>
- Dahlbom, D. A., Brooks, F. T., Wilson, M. S., Chi, S., Kolesnikov, A. I., Stone, M. B., Cao, H., Li, Y. W., Barros, K., Mourigal, M., & others. (2024). Quantum-to-classical crossover in generalized spin systems: Temperature-dependent spin dynamics of FeI_2 . *Physical Review B*, 109(1), 014427. <https://doi.org/10.1103/PhysRevB.109.014427>
- Dahlbom, D. A., Miles, C., Zhang, H., Batista, C. D., & Barros, K. (2022). Langevin dynamics of generalized spins as $\text{SU}(N)$ coherent states. *Physical Review B*, 106(23), 235154. <https://doi.org/10.1103/PhysRevB.106.235154>

- Dahlbom, D. A., Thomas, J., Johnston, S., Barros, K., & Batista, C. D. (2024). Classical dynamics of the antiferromagnetic Heisenberg $S = \frac{1}{2}$ spin ladder. *Physical Review B*, *110*(10), 104403. <https://doi.org/10.1103/PhysRevB.110.104403>
- Dahlbom, D. A., Zhang, H., Laraib, Z., Pajerowski, D. M., Barros, K., & Batista, C. D. (2025). Renormalized classical theory of quantum magnets. *Physical Review B*, *112*(13), 134432. <https://doi.org/10.1103/x7c2-x8p6>
- Dahlbom, D. A., Zhang, H., Miles, C., Bai, X., Batista, C. D., & Barros, K. (2022). Geometric integration of classical spin dynamics via a mean-field Schrödinger equation. *Physical Review B*, *106*(5), 054423. <https://doi.org/10.1103/PhysRevB.106.054423>
- Danisch, S., & Krumbiegel, J. (2021). Makie.jl: Flexible high-performance data visualization for Julia. *Journal of Open Source Software*, *6*(65), 3349. <https://doi.org/10.21105/joss.03349>
- Do, S.-H., Zhang, H., Dahlbom, D. A., Williams, T. J., Garlea, V. O., Hong, T., Jang, T.-H., Cheong, S.-W., Park, J.-H., Barros, K., & others. (2023). Understanding temperature-dependent SU(3) spin dynamics in the $S=1$ antiferromagnet $\text{Ba}_2\text{FeSi}_2\text{O}_7$. *Npj Quantum Materials*, *8*(1), 5. <https://doi.org/10.1038/s41535-022-00526-7>
- Evans, R. F. L., Fan, W. J., Churemart, P., Ostler, T. A., Ellis, M. O. A., & Chantrell, R. W. (2014). Atomistic spin model simulations of magnetic nanomaterials. *Journal of Physics: Condensed Matter*, *26*(10), 103202. <https://doi.org/10.1088/0953-8984/26/10/103202>
- Hahn, S., Granroth, G., Peterson, P., & Whitfield, R. (2024). SpinWaveGenie. In *GitHub repository*. GitHub. <https://github.com/SpinWaveGenie/SpinWaveGenie>
- Hall, S. R., Allen, F. H., & Brown, I. D. (1991). The crystallographic information file (CIF): A new standard archive file for crystallography. *Foundations of Crystallography*, *47*(6), 655–685. <https://doi.org/10.1107/S010876739101067X>
- Hester, J., & Richard, B. (2024). CrystalInfoFramework. In *GitHub repository*. GitHub. <https://github.com/jamesrhester/CrystalInfoFramework.jl>
- Kim, C., Kim, S., Park, P., Kim, T., Jeong, J., Ohira-Kawamura, S., Murai, N., Nakajima, K., Chernyshev, A. L., Mourigal, M., & others. (2023). Bond-dependent anisotropy and magnon decay in cobalt-based Kitaev triangular antiferromagnet. *Nature Physics*, *19*(11), 1624–1629. <https://doi.org/10.1038/s41567-023-02180-7>
- Lane, H., Zhang, H., Dahlbom, D. A., Quinn, S., Somma, R., Mourigal, M., Batista, C. D., & Barros, K. (2024). Kernel polynomial method for linear spin wave theory. *SciPost Physics*, *17*(5), 145. <https://doi.org/10.21468/SciPostPhys.17.5.145>
- Lee, M., Schönemann, R., Zhang, H., Dahlbom, D., Jang, T.-H., Do, S.-H., Christianson, A. D., Cheong, S.-W., Park, J.-H., Brosha, E., & others. (2023). Field-induced spin level crossings within a quasi-XY antiferromagnetic state in $\text{Ba}_2\text{FeSi}_2\text{O}_7$. *Physical Review B*, *107*(14), 144427. <https://doi.org/10.1103/PhysRevB.107.144427>
- Legros, A., Zhang, S. S., Bai, X., Zhang, H., Dun, Z., Phelan, W. A., Batista, C. D., Mourigal, M., & Armitage, N. P. (2021). Observation of 4- and 6-magnon bound states in the spin-anisotropic frustrated antiferromagnet FeI_2 . *Physical Review Letters*, *127*(26), 267201. <https://doi.org/10.1103/PhysRevLett.127.267201>
- Li, B. (2024). pyLiSW. In *GitHub repository*. GitHub. <https://github.com/bingli621/pyLiSW>
- Mogensen, P., & Riseth, A. (2018). Optim: A mathematical optimization package for Julia. *Journal of Open Source Software*, *3*(24). <https://doi.org/10.21105/joss.00615>
- Müller, G. P., Hoffmann, M., DiBelkamp, C., Schürhoff, D., Mavros, S., Sallermann, M., Kiselev, N. S., Jónsson, H., & Blügel, S. (2019). Spirit: Multifunctional framework for atomistic spin simulations. *Physical Review B*, *99*(22), 224414. <https://doi.org/10.1103/PhysRevB.99.224414>

- Muniz, R. A., Kato, Y., & Batista, C. D. (2014). Generalized spin-wave theory: Application to the bilinear–biquadratic model. *Progress of Theoretical and Experimental Physics*, 2014(8), 083101. <https://doi.org/10.1093/ptep/ptu109>
- Na, W., Park, P., Oh, S., Kim, J., Scheie, A., Tennant, D. A., Lee, H. C., Park, J.-G., & Cheong, H. (2024). Direct observation and analysis of low-energy magnons with Raman spectroscopy in atomically thin NiPS₃. *ACS Nano*, 18(31), 20482–20492. <https://doi.org/10.1021/acs.nano.4c04824>
- Nagl, J., Flavián, D., Hayashida, S., Povarov, K. Y., Yan, M., Murai, N., Ohira-Kawamura, S., Simutis, G., Hicken, T. J., Luetkens, H., & others. (2024). Excitation spectrum and spin Hamiltonian of the frustrated quantum Ising magnet Pr₃BWO₉. *Physical Review Research*, 6(2), 023267. <https://doi.org/10.1103/PhysRevResearch.6.023267>
- Paddison, J. A. M. (2023). Spinteract: A program to refine magnetic interactions to diffuse scattering data. *Journal of Physics: Condensed Matter*, 35(49), 495802. <https://doi.org/10.1088/1361-648X/acf261>
- Paddison, J. A. M., Zhang, H., Yan, J., Cliffe, M. J., McGuire, M. A., Do, S.-H., Gao, S., Stone, M. B., Dahlbom, D. A., Barros, K., & others. (2024). Cubic double perovskites host noncoplanar spin textures. *Npj Quantum Materials*, 9(1), 48. <https://doi.org/10.1038/s41535-024-00650-6>
- Park, Pyeongjae, Cho, W., Kim, C., An, Y., Iida, K., Kajimoto, R., Matin, S., Zhang, S.-S., Batista, C. D., & Park, J.-G. (2025). Spin dynamics of triple-q magnetic orderings in a triangular lattice: Implications for multi-q orderings in general two-dimensional lattices. *Physical Review X*, 15(3), 031032. <https://doi.org/10.1103/y9ly-4kld>
- Park, P., Cho, W., Kim, C., An, Y., Kang, Y.-G., Avdeev, M., Sibille, R., Iida, K., Kajimoto, R., Lee, K. H., & others. (2023). Tetrahedral triple-Q magnetic ordering and large spontaneous Hall conductivity in the metallic triangular antiferromagnet Co_{1/3}TaS₂. *Nature Communications*, 14(1), 8346. <https://doi.org/10.1038/s41467-023-43853-4>
- Park, P., Ghioldi, E. A., May, A. F., Kolopus, J. A., Podlesnyak, A. A., Calder, S., Paddison, J. A. M., Trumper, A. E., Manuel, L. O., Batista, C. D., & others. (2024). Anomalous continuum scattering and higher-order van Hove singularity in the strongly anisotropic $S = \frac{1}{2}$ triangular lattice antiferromagnet. *Nature Communications*, 15(1), 7264. <https://doi.org/10.1103/PhysRevResearch.6.033184>
- Park, P., Sala, G., Pajeroski, D. M., May, A. F., Kolopus, J. A., Dahlbom, D. A., Stone, M. B., Halász, G. B., & Christianson, A. D. (2024). Quantum and classical spin dynamics across temperature scales in the $S = \frac{1}{2}$ Heisenberg antiferromagnet. *Physical Review Research*, 6(3), 033184. <https://doi.org/10.1103/PhysRevResearch.6.033184>
- Petit, S., & Damay, F. (2016). SpinWave, a software dedicated to spin wave simulations. *Neutron News*, 27(4), 27–28. <https://doi.org/10.1080/10448632.2016.1233020>
- Rotter, M. (2004). Using McPhase to calculate magnetic phase diagrams of rare earth compounds. *Journal of Magnetism and Magnetic Materials*, 272, E481–E482. <https://doi.org/10.1016/j.jmmm.2003.12.1394>
- Scheie, A., Park, P., Villanova, J. W., Granroth, G. E., Sarkis, C. L., Zhang, H., Stone, M. B., Park, J.-G., Okamoto, S., Berlijn, T., & others. (2023). Spin wave Hamiltonian and anomalous scattering in NiPS₃. *Physical Review B*, 108(10), 104402. <https://doi.org/10.1103/PhysRevB.108.104402>
- Swendsen, R. H., & Wang, J.-S. (1986). Replica Monte Carlo simulation of spin-glasses. *Physical Review Letters*, 57(21), 2607. <https://doi.org/10.1103/PhysRevLett.57.2607>
- Togo, A., Shinohara, K., & Tanaka, I. (2024). Spglib: A software library for crystal symmetry search. *Science and Technology of Advanced Materials: Methods*, 4(1), 2384822. <https://doi.org/10.1002/stam.10001>

[//doi.org/10.1080/27660400.2024.2384822](https://doi.org/10.1080/27660400.2024.2384822)

- Toth, S., & Lake, B. (2015). Linear spin wave theory for single-Q incommensurate magnetic structures. *Journal of Physics: Condensed Matter*, 27(16), 166002. <https://doi.org/10.1088/0953-8984/27/16/166002>
- Wang, F., & Landau, D. P. (2001). Efficient, multiple-range random walk algorithm to calculate the density of states. *Physical Review Letters*, 86(10), 2050. <https://doi.org/10.1103/PhysRevLett.86.2050>
- Watson, G. R., Cage, G., Fortney, J., Granroth, G. E., Hughes, H., Maier, T., McDonnell, M., Ramirez-Cuesta, A., Smith, R., Yakubov, S., & others. (2022). Calvera: A platform for the interpretation and analysis of neutron scattering data. *Smoky Mountains Computational Sciences and Engineering Conference*, 137–154. https://doi.org/10.1007/978-3-031-23606-8_9
- Weber, T., Georgii, R., & Böni, P. (2016). Takin: An open-source software for experiment planning, visualisation, and data analysis. *SoftwareX*, 5, 121–126. <https://doi.org/10.1016/j.softx.2016.06.002>
- Zhang, H., & Batista, C. D. (2021). Classical spin dynamics based on SU(N) coherent states. *Physical Review B*, 104(10), 104409. <https://doi.org/10.1103/PhysRevB.104.104409>
- Zhang, H., & Lin, S. Z. (2024). Multipolar skyrmion crystals in non-Kramers doublet systems. *Physical Review Letters*, 133(19), 196702. <https://doi.org/10.1103/PhysRevLett.133.196702>
- Zhang, H., Wang, Z., Dahlbom, D. A., Barros, K., & Batista, C. D. (2023). CP² skyrmions and skyrmion crystals in realistic quantum magnets. *Nature Communications*, 14(1), 3626. <https://doi.org/10.1038/s41467-023-39232-8>