

PeiYu CAI

PhD Candidate in Physics | Computational Magnetism & Spintronics

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Education

March 2023 ~ (Present)	PhD Student at University of Edinburgh, UK Supervised by: Prof. Elton J. G. Santos Research Project: Multi-scale approach for spin dynamics on Two-Dimensional (2D) Magnetic Materials and Applications.
October 2022	Master (MSc) in Physics at Imperial College London, UK Classification: Distinction (1st Class Honors) Master's Thesis: Spin Torque Nano-Oscillators (STNO) and possible applications in artificial neural networks for image processing and sound recognition
May 2021	Bachelor of Science at University of Central Florida, US Dual Major: Physics, Mathematics GPA: 3.9/4.0 in Physics, 3.75/4.0 Overall

Funding, Scholarships & Awards

- Conference Travel Support (\$1,000) – Magnetism and Magnetic Materials (MMM) 2026 Conference.
- PhD Scholarship – China Scholarship Council (CSC), 2022 (Full tuition waiver and comprehensive monthly living stipend).
- Dean's List – University of Central Florida (Awarded 6 times: Spring 2018, Fall 2018, Spring 2019, Fall 2019, Spring 2020, Spring 2021).

Research Experience

University of Edinburgh – PhD Researcher (March 2023 – Present)

- Utilize advanced multi-scale computational frameworks, combining atomistic spin dynamics and micromagnetic simulation techniques, to reveal the intrinsic properties of 2D van der Waals (vdW) magnets.
- Investigate low-dimensional magnetic architectures including $\text{Cr}_2\text{Ge}_2\text{Te}_6$ (CGT), $\text{Cr}_2\text{Si}_2\text{Te}_6$ (CST), Fe_3GeTe_2 (FGT-312), Fe_3GaTe_2 (FGaT), and CrTe_2 .
- Reproduce complex magnetic phases and spin structures from numerical modeling to validate experimental discoveries and clarify the underlying microscopic physical mechanisms.

University of Central Florida – Undergraduate Research Assistant (Aug 2019 – May 2021)

- Contributed to research in wave functions for high-symmetry, two-dimensional microstrip antennas and boxes.
- Designed a program using Mathematica that helped analyzing symmetry patterns in different modes of wave function, increased efficiency for analyzing lower order nodes and made analyzing higher order nodes possible.
- Identified C_{3v} wave function symmetries in equilateral triangular boundary systems and implemented 1D or 2D representations accordingly so that the outcome is legible to readers.
- Verified solutions for circular boundary problems and the coefficients calculated by other members, which is crucial for the correctness of plots.

Publications

1. Xi Zhang, Jingcheng Zhou, ..., **PeiYu Cai**, ..., Elton J. G. Santos, Jiun-Haw Chu, Chunhui Rita Du, and Hailong Wang. **"Self-Integrated Quantum Imaging of an All-van der Waals Spin-Orbit Torque System."** *Nature Communications*, 2026. DOI: 10.1038/s41467-026-74178-7.
 - Contribution: Disentangled the specific contributions of field-like and damping-like torques during deterministic switching and analyzed the critical current densities to clarify the interplay of SOT and STT in Fe₃GaTe₂/hBN heterostructures.
2. Jixiang Huang[†], Tongji Zhu[†], **PeiYu Cai**[†], ..., Wanjun Jiang, Jing Tao, Shiming Lei, Pavel Parchinskiy, Lingfei Wang, Wei Niu, Elton J.G. Santos, Xiaoqian Zhang, Peng Li. **"Room-Temperature Skyrmionic Synapse in 2D Ferromagnet Operating via Collective Spin Texture Transformation."** *Advanced Materials*, e20288 (2026). DOI: 10.1002/adma.202520288.
 - Contribution: Led the theoretical validation by employing GPU-accelerated micromagnetic simulations to reproduce the current-driven skyrmion-to-stripe phase transformation; quantified topological charge annihilation and identified the transition as a demagnetization-driven, SOT-assisted thermodynamic relaxation process.
3. Charlie W. F. Freeman, Woohyun Cho, Paul S. Keatley, **PeiYu Cai**, Elton J. G. Santos, Robert J. Hicken, H. Yang, Hidekazu Kurebayashi, Murat Cubukcu, and Maciej Dabrowski. **"Laser-Induced Topological Toggle Switching at Room Temperature in the van der Waals Ferromagnet."** *npj Spintronics*, 4, 24 (2026). DOI: 10.1038/s44306-026-00139-x.
 - Contribution: Modeled the thermodynamics of topological switching and demonstrated the complex interplay between thermal fluctuations and external fields during skyrmion formation, validating the physical mechanism for all-optical toggle switching.
4. Sang-Eon Lee, Yue Li, Yeonkyu Lee, W. Kice Brown, **PeiYu Cai**, ..., Elton J. G. Santos, Jeehoon Kim, Charudatta M. Phatak, Vadym Kulichenko, and Luis Balicas. **"Local Inversion Symmetry Breaking and Thermodynamic Evidence for Ferrimagnetism**

in Fe₃GaTe₂." *ACS Nano*, 19, 28702–28718 (2025). DOI: 10.1021/acsnano.5c08312.

- Contribution: Investigated the impacts of localized symmetry breaking on topological spin configurations and successfully differentiated Néel and Bloch-hybrid skyrmions via parameter tuning to match experimental Lorentz TEM data.
5. Jennifer Garland, John Fullerton, **PeiYu Cai**, Rabindra Basnet, Santosh Karki Chhetri, Jin Hu, Elton J. G. Santos, Yue Li, Charudatta Phatak, and Amanda Petford-Long. **"Thickness-Dependent Skyrmion Evolution in During Magnetization Reversal."** *Advanced Functional Materials*, e18239 (2025). DOI: 10.1002/adfm.202518239.
 - Contribution: Executed comprehensive energy density analysis across varied system thicknesses to quantify confinement effects on topological stability, establishing the theoretical thickness thresholds for stable skyrmion formation.
 6. Xiaoqian Zhang, Yue Li, ..., **PeiYu Cai**, Elton J. G. Santos, Charudatta Phatak, Wei Zhang, Nan Gao, Wei Niu, Guang Bian, Peng Li, Dapeng Yu, and Shibing Long. **"Epitaxial Growth of Large-Scale 2D Films on Amorphous Silicon Wafers With Low Thermal Budget."** *Advanced Materials*, 2311591 (2024). (Featured on Journal Cover) DOI: 10.1002/adma.202311591.
 - Contribution: Conducted micromagnetic simulations to reveal the critical role of interfacial Dzyaloshinskii-Moriya Interaction (DMI) in stabilizing skyrmions within the CrTe₂ system, providing numerical estimations for the required DMI strength.
 7. Joseph R. Rain[†], **PeiYu Cai**[†], Alexander Baekey[†], Matthew A. Reinhard, Roman I. Vasquez, Andrew C. Silverman, Christopher L. Cain, and Richard A. Klemm. **"Wave functions for high-symmetry, two-dimensional microstrip antennas and boxes."** *Physical Review A*, 104, 062205 (2021). DOI: 10.1103/PhysRevA.104.062205.

Conferences & Presentations

- **Poster Presentation** | *Micromagnetic Investigation of Thickness-Dependent Skyrmion Evolution and Pinning In Fe₃GaTe₂* **Intermag 2026 Conference** | April 2026
 - *Abstract:* Presented micromagnetic frameworks of containing structural thickness variations to replicate Cryo-LTEM observations. Validated how 75 nm regimes stabilize high-density skyrmion lattices that transition into faceted patch domains bounded by 360° domain walls during field reversal. Pinpointed abrupt demagnetization-field gradients at step edges as the foundational pinning mechanism, detailing a predictive layout for routing domain walls in vdW devices.
- **Oral Presentation** | *Thickness-Dependent Skyrmion Evolution in during Magnetization Reversal* **IEEE ATC_ATG 2025 Conference** | November 2025
 - *Abstract:* Investigated magnetic reversal states across exfoliated structural flakes via in-situ cryo-LTEM and matching micromagnetic runs. Characterized phase space shifts among stripe structures, topological skyrmions, and

faceted patch geometries, emphasizing severe local pinning at cross-sectional steps governed by magnetic anisotropy, external fields, and demagnetization profiles.

- **Invited Tutorial** | *Tutorial: Simulating 2D van der Waals Magnets with VAMPIRE* **VAMPIRE Workshop 2023**, University of York, UK | October 2023
 - *Abstract:* Delivered an invited technical masterclass outlining methodologies for constructing atomistic representations of 2D vdW magnets utilizing the VAMPIRE toolkit. Covered workflow initializations, parameter tuning/benchmarking, and physical interpretation of magnetic phases. The lecture series was published to YouTube as an open-access training resource for the international spintronics community.

Professional & Teaching Experience

University of Edinburgh, UK — Graduate Teaching Assistant | Sep 2023 – Present

- Facilitate and present technical instruction across multiple advanced undergraduate physics seminars and computational physics laboratories.
- Mentor students in evaluating data acquisition architectures, establishing error propagation models, and resolving numerical bottlenecks within physics simulations.

University of Central Florida, US — Learning Assistant | January 2020 – May 2020

- Constructed and led interactive recitations, problem-solving clinics, and visual physics demonstrations to break down complex electromagnetic and mechanical concepts for introductory students.

Deloitte (Hong Kong S.A.R.) — IT Audit Summer Intern | June 2019 – July 2019

- Assisted full-time within the enterprise IT Audit Department, compiling formal service and advisory proposals for commercial client acquisition.
- Conducted rigorous technical audits of client corporate financial ledgers and digital security infrastructures to verify regulatory compliance.
- Executed an independent investigative study regarding optimization methodologies within corporate system auditing frameworks.
- Onboarded and structured training routines for incoming department personnel to accelerate team integration into day-to-day data pipelines.

Tongfang Kontafarma Holdings Ltd (Hong Kong S.A.R.) — Corporate & Financial Analyst Intern | July 2017

- Completed a structured, one-month immersion focused on multinational corporate infrastructure, analyzing operational datasets and core balance sheets.
- Synthesized financial data trends to evaluate management workflows and assisted administrative teams in executing internal office operational duties.

Scientific & Technical Skills

- **Computational Physics & Modeling:** Expert in Multi-scale Spin Dynamics modeling;

proficient in Atomistic simulations via the VAMPIRE package and Micromagnetic modeling using MUMAX3.

- **Data Analysis & Scientific Visualization:** Advanced post-processing of magnetization configuration arrays; highly proficient in ParaView, Povray, MATLAB, Mathematica, and Gnuplot.
- **Programming Languages:** Python (NumPy, Pandas, SciPy), C, Java, and Wolfram Mathematica.
- **High-Performance Computing (HPC):** Extensive experience deploying, running, and managing complex workloads on supercomputing clusters, including the HPE Cray architecture on ARCHER2, CentOS on Cirrus, and Imperial College HPC nodes.
- **Hardware & Experimental Electronics:** Proficient with laboratory oscilloscopes, digital multimeters, and troubleshooting custom analog circuitry containing operational amplifiers, transistors, diodes, and voltage regulators.
- **Statistical Data Processing:** Skilled in scientific statistical analysis including Gauss error propagation modeling for systematic errors, and numerical interpolations with Binomial, Poisson, and Gaussian probability distribution functions.
- **Methodological Frameworks:** Strategic employment of AI-driven insights to navigate complex computational math problems and optimize the high-performance computing research lifecycle.
- **Financial Computing:** Competent in executing structural data analysis and optimization formulas using Microsoft Excel.

Languages

- Chinese Mandarin: Native Speaker.
- English: Full Professional Proficiency / Fluent.