Johan Yapo

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SUMMARY

- Computational Chemistry and Materials Science expert with over 5 years of experience leveraging Density Functional Theory (VASP) and advanced AI/ML techniques to accelerate novel materials discovery, with a focus on energy materials, electro-catalysts, and magnetically active crystalline compounds, and recently, applications in biosensing devices. Proven track record of 7 peer-reviewed publications and presentations, and 2 fellowship awards, demonstrating a strong capability to bridge computational insights with real-world applications in materials design.

EDUCATION

PhD in Physical Chemistry June 2025
University of California Riverside (UCR)
- Dissertation title: "*Application of Machine Learning Towards Discovering Magnetic Borides*"

BSc. in Specialized Chemistry May 2017
University of Illinois Urbana-Champaign (UIUC)

TECHNICAL SKILLS

Programming: Python (NumPy, SciPy, MatPlotLib, Pandas, PyTorch, scikit-learn), Bash, Java, SQL, Git
Libraries & APIs: Pytorch, TensorFlow, Pymatgen, MatMiner, SHapley Additive exPlanations (SHAP), REST
Machine Learning: Neural Networks, XGBoost, Random Forest, Cheminformatics, Materials Informatics (Pymatgen, JARVIS-ML, CBFV)
Computational Chemistry: Density Functional Theory (DFT), Spin-Orbit Coupling (SOC), Surface Slab Modeling, Electronic Structure Analysis, Crystal Orbital Hamilton Population (COHP), Bader Charge Analysis
Software/Tools: VASP, LOBSTER, SLURM, Github, Globus Data Transfer, Jupyter, Gaussian, AMBER
Experimental: Arc-melting, X-ray diffraction (XRD), FT-IR, X-ray fluorescence, GC-MS, UV-VIS spectroscopy

RESEARCH WORK EXPERIENCE

Graduate Student Researcher, UCR September 2019 to June 2025
Project: Machine Learning Predictions of the Magnetic Properties of Inorganic Materials
- Led the development of AI/ML methods to accelerate the discovery and design of novel magnetic inorganic materials, focusing on predicting magnetic properties and generating actionable insights for materials development.
- Curated a comprehensive dataset of 8,438 inorganic materials from the Materials Project Database, strategically extracting key chemical and structural descriptors for training advanced AI and Machine Learning models in a materials informatics workflow.
- Engineered and validated high-performance ML and AI algorithms, including Graph Neural Networks (GNNs), Sequential Neural Networks (SNNs), XGBoost, and Random Forest models, achieving correlation coefficients of 0.90, significantly exceeding published benchmarks for similar materials prediction tasks
- Executed high-throughput computational predictions on over 60,000 theoretical compounds, identifying 544 promising candidates for novel magnetic borides, directly contributing to the data-driven design of functional materials relevant to advanced energy applications.

Project: DFT studies on Earth-Abundant Transition Metal Borides (TMBs) as electro-catalysts for Hydrogen Evolution Reaction (HER) in Fuel Cells
- Contributed to an interdisciplinary team conducting ab-initio simulations to analyze catalytically active sites of inorganic materials relevant to energy applications.
- Bridged computational predictions with experimental efforts by providing critical computational insights that directly guided the synthesis and characterization of electro-catalysts, leading to 6 peer-reviewed publications, including a contribution to *ACS Materials Letters*.

- Developed a methodology to link structure-property relationships of crystalline materials to catalytic enhancement by calculating Hydrogen adsorption sites via VASP software for 10 Transition Metal Borides (TMBs), creating a robust dataset for inorganic electro-catalysts.
- Pioneered vacancy engineering as a novel design strategy for developing high-efficiency HER electro-catalysts through in-depth DFT and COHP bond analysis, identifying key metal-metal, metal-boron, and boron-boron bond characteristics.

Volunteer Research Associate, University of Illinois at Chicago (UIC) May 2025 to present

- Co-developed a noninvasive biosensing device in a collaborative team of bioengineers and biochemists to enable early detection of pancreatic cancer.
- Engineered and deployed a machine learning pipeline utilizing Support Vector Machine (SVM) and Neural Network models to predict the risk of pancreatic cancer based on electrical impedance data of target biomarkers for biosensing applications.
- Expanded training dataset for neural networks by generating 3,000 synthetic data points using generative AI principles, leading to improved accuracy in pancreatic cancer screening.

WORK EXPERIENCE

Course Developer and Instructor, UCR Office of Diversity, Equity, and Inclusion January 2024 to June 2024

- Demonstrated leadership and collaboration skills as a DEI practitioner, advancing STEM accessibility through the application of inclusive practices and cultural competence.
- Worked as part of a cross-functional team with the UCR School of Education and Office of DEI to develop curriculum and content for a new online DEI course tailored to international graduate students.
- Developed and delivered instructional materials to teach crucial DEI concepts to students with minimal prior experience, strengthening communication and educational outreach skills.

Teaching Assistant, UCR September 2020 to August 2024

- Created tailored lesson plans, lectures, and in-class activities for chemistry courses, emphasizing inclusive pedagogical practices to support first-generation college students.
- Demonstrated leadership and cross-functional collaboration skills as a DEI practitioner, advancing STEM accessibility and fostering an equitable research environment.
- Developed and implemented a rubric for teaching assistants to promote inclusive practices and equitable participation in introductory STEM laboratory courses, resulting in improved student engagement and achievement.

Quality Control Technician II, Chemtool Incorporated June 2017 to August 2019

- Applied meticulous attention to detail and instrument maintenance proficiency through regular calibrations and upkeep of sophisticated analytical equipment.
- Rigorously tested aerospace-grade lubricants against stringent specifications to ensure compliance with quality standards.
- Managed a fast-paced workflow with a cross-functional team of chemists and engineers, performing up to 30 daily tests to ensure the quality and compliance of lubricants.

PUBLICATIONS & PRESENTATIONS

Yapo, J. A. Application of machine learning towards discovering magnetic borides. PhD thesis, Univ. of California, Riverside (2025). Available at https://escholarship.org/uc/item/0m58d8sj

Kim, S. B., **Yapo, J. A.**, Yasuhara, A., Yubuta, K. & Fokwa, B. P. T. Vanadium-stabilized MoB nanoparticles enable hydrogen evolution at industry-relevant high current densities. *Small* e2412693 (2025) doi:10.1002/smll.202412693. **(co-first author)**

Lee, E., **Yapo, J. A.**, Bhupathy, A., Mentzel, T., Yin, X., & Fokwa, B. P. T. (2025) Volcano-Like Diboride Solid Solutions: Synergistic Antibonding and Vacancy Effects for Superior High-Current-Density Hydrogen Evolution. ACS Energy Letters. **(co-first author)** [Just Accepted]

Yapo, J. A. (2023). *Harnessing the power of machine learning for the discovery and understanding of novel magnetic metal borides* [Poster #1513]. Presented at the American Chemical Society (ACS) National Meeting & Expo. Retrieved from https://acs.digitellinc.com/b/sp/johan-yapo-170185

Rezaie, A. A., Lee, E., Luong, D., **Yapo, J. A.**, & Fokwa, B. P. T. (2022). $Fe_5Ge_2Te_2$: Iron-rich Layered Chalcogenide for Highly Efficient Hydrogen Evolution. Zeitschrift für anorganische und allgemeine Chemie, 648(10), e202200066. https://doi.org/10.1002/zaac.202200066 **(co-first author)**

Rezaie, A. A., Lee, E**., Yapo, J. A.,** & Fokwa, B. P. T. (2021). Highly Active and Abundant MAB Phases $Ni_{n+1}ZnB_n$ (n=1,2) Toward Hydrogen Evolution. *Advanced Energy and Sustainability Research, 2(5), 2100052*. https://doi.org/10.1002/aesr.202100052 **(co-first author)**

Rezaie, A. A., Lee, E., Luong, D., **Yapo, J. A.**, & Fokwa, B. P. T. (2021). Abundant Active Sites on the Basal Plane and Edges of Layered van der Waals Fe_3GeTe_2 for Highly Efficient Hydrogen Evolution. *ACS Materials Letters, 3(3), 313–319*. https://doi.org/10.1021/acsmaterialslett.1c00048

AWARDS

- Alliances for Graduate Education and the Professoriate (AGEP) NSF Funding Award September 2021
- Advancing Faculty Diversity Award, UCR Department of Chemistry September 2024

CERTIFICATIONS

- Chancellor's "Making Excellence Inclusive" DEI Certificate Program, UCR June 2023
- IBM Data Science by IBM on Coursera March 2025