CURRENT RESEARCH (as of April 6, 2024)

Advisor: Dr. Zi-Kui Liu, P. Enright Distinguished Professor August 2019 — Present
The Pennsylvania State University, USA

- (Lead Developer) **ULtrahigh TEmperature Refractory Alloys (ULTERA) Database** (**ultera.org**) containing 2,800 unique HEAs with 6,300 property-datapoints from 540 literature publications; optimized for ML inverse design (**Article**) combined with extensive data curation and quality assurance using abnormal data detection techniques.
- (Lead Dev) **pySIPFENN: python toolset for Structure-Informed Property and Feature Engineering with Neural Networks** with transfer learning capabilities (including automated model tuning with OPTIMADE API) and physics-based efficiency optimizations for ordered, dilute, and random solid solutions.
  Detailed in (**Documentation**) (**GitHub**) (**2022 Paper**) (**2024 Paper**) (**NN Models**)
- (Lead Dev) **nimplex: Efficient Generation of Grids and Traversal Graphs in Compositional Spaces** towards exploration and path planning across disciplines, from functionally graded materials to financial modeling, using my novel algorithm (**Paper**)
- (Lead Dev) **nimCSO: nim Composition Space Optimization** for design element selection for ML from compositionally complex datasets with millions of points (**Paper**)
- (Lead Dev) **Material-Property-Descriptor Database (MPDD)** for rapid ML model deployment on millions of atomic structures (**Description**) (**in OPTIMADE Paper**)
- (Lead Dev) **Pure Data Driven Structure Prediction (crystALL)** combining MPDD's Big Data from DFT with high-throughput substitutions, stability predictions, candidate selection, and DFT+experiment validation. Demonstrated in the identification of new atomic structures in Nd-Bi (**Acta Mat.**) and Al-Fe (**Nature SR**) systems.
- (Lead Dev) **Materials data curation and abnormality detection in compositionally complex materials (PyQAlloy.ultera.org) and DFT Databases**. Extended by research in techniques combining datasets from different methods or settings.
- Additional software I worked on in the past is listed at: (**software.phaseslab.org**)

Lawrence Livermore National Lab: MaCI 2022, CCMS 2023 & Remote Collaboration (Lanthanides and Actinides Computational Group) June 2022 - Present
Materials Science Division at Lawrence Livermore National Lab, USA

(Lead Developer) The engine behind *MAP* infrastructure for high-throughput **complete computational exploration of 2-9 component HEAs** in a 20 component space.

RECENT AND UPCOMING CONFERENCE PRESENTATIONS

CIMTEC 2024 (Montecatini Terme, Italy, June 2024) **(Invited Talk)**

MaRDA (Virtual, Feb 2024) **(Data Platforms Session)**

Intellegens *DataBites* (Cambridge, UK, Nov 2023) **(Company-Wide Invited Talk)**
Alloy Data Processing, Validation, Abnormality Detection

CALPHAD 2023 (Cambridge, MA, June 2023) **(Talk)**
Creating an Efficient Alloy Database Infrastructure and Detecting Abnormal Data in ULTERA Project

E-MRS 2023 (Strasbourg, France, May 2023) **(Talk)**
ULTERA Database Infrastructure and Abnormal Data Detection

TMS 2023 (San Diego, CA, March 2023) **(Three Talks)**
ULtrahigh TEmperature Refractory Alloys (ULTERA) Database and Data Quality Assurance & (LLNL) High-Throughput CALPHAD Exploration of Multi-Principal Element Alloy (MPEA) Space for Targeted Properties and Structure

IMAT 2022 **(Talk)**

MRS Spring 2022 **(Two Talks)**

MRS Spring 2021 **(Talk)**

MRS Fall 2019 **(Poster)**

MRS Fall 2018 **(Poster)**

CALPHAD 2022 **(Talk)**

IMAT 2021 **(Invited Talk)**

MRS Spring/Fall 2020 **(Poster and Talk)**

MS&T 2018 **(Talk)**

Adam M. Krajewski

Ph.D. Candidate
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Phases Research Lab

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EDUCATION

PhD Candidate in Materials Science and Engineering with Computational Materials Doctoral Minor
The Pennsylvania State University, USA
2019—Present

BSE in Materials Science and Engineering with AI and Physics Minors
Case Western Reserve University, USA
2015-2019

RECENT AWARDS

Throwers Cambridge Fellowship (09/2023)
NSF CALPHAD Scholarship (06/2023)
5x iMATSE Travel Award (2019-23)
Industry Best Poster Award at PSU Research Showcase (10/2022)
Best Talk Award at MRS Spring'22 SF09 (05/2022)
STT CALPHAD Scholarship (02/2020)
Leichliter Graduate Fellowship (2019-2020)
Kent R. van Horn Scholarship (2016-2019)

RESEARCH INTERESTS

Materials Discovery
Artificial Intelligence
High Performance Computing
Complex Database Design
Machine Learning
Refractory High Entropy Alloys
Abnormal Data Detection
Comp. Thermodynamics
Functionally Graded Materials

TEACHING EXPERIENCE

Computational Thermodynamics, PSU **Fall 2023**
Teaching Assistant (volunteered) - I gave workshop-style guest lectures open-sourced at **this link**.

Phase Relations in Materials Systems, PSU **Spring 2021**
Teaching Assistant (volunteered)

Phase Relations in Materials Systems, PSU **Spring 2020**
Teaching Assistant (volunteered) - I gave several lectures and prepared several other.

Role of Materials in Energy and Sustainability, CWRU **Spring 2019**
I took the class one-on-one and **revised all lecture materials**.

Mathematical and Computational Methods for Materials Science, CWRU **Spring 2019**
Teaching Assistant (volunteered) - I gave one 2h lecture every week, designed by me from scratch.

Mathematical and Computational Methods for Materials Science, CWRU **Spring 2018**
Teaching Assistant (volunteered) - I was the first non-PhD to TA this course at CWRU. I gave several lectures and helped update curriculum.

WORK EXPERIENCE

CCMS Internship at Lawrence Livermore National Laboratory **Summer 2023**
Lanthanides and Actinides Computational Group in MSD-PLS

MaCI Internship at Lawrence Livermore National Laboratory **Summer 2022**
Lanthanides and Actinides Computational Group in MSD-PLS

Research Assistant at The Pennsylvania State University **Fall 2019 - Present**
Research-only appointment at the Phases Research Lab (**phaseslab.org**) plus volunteer teaching work in related courses.

Self-Employed Sailboat Captain (Greece/Croatia) **Summers of 2013 - 2019**
I hold a captain's license since 2013 and I've spent seven summers organizing 35-50ft sailboat cruises on the Atlantic and Mediterranean. This gave me 4,000+h of leadership and management experience, including during unexpected and high-stress conditions.

OTHER SIGNIFICANT EXPERIENCES

Visiting PhD Student at Gonville&Caius (University of Cambridge) **Fall 2023**
In November/December 2023, I've had the pleasure of being invited to Cambridge, UK by the Gonville and Caius College. During my time there, I've had numerous discussions, gave lectures on my research, and wrote a nice paper in the College's library.

Funding Advocacy in the United States Congress **Springs of 2018, 2019, 2023**
I've traveled to Washington, DC on 3 advocacy trips sponsored by professional organizations (ASM, TMS, ACerS, AIST) and had a chance to discuss impact of my research with numerous senators, representatives, and staffers.

PROGRAMMING LANGUAGES

+ some: C, Java, R, AVR BASIC/assembler, and I like learning new ones.

RELEVANT SKILLS

+ some: CALPHAD, BBO techniques, and ab-initio/DFT.

Beginner Intermediate Advanced

ACADEMIC INTERESTS

Accessible Teaching Methods
Additive Manufacturing
Ab-Initio Calculations
Novel Concepts for Space Exploration
Casual Mathematics
Formal Logic
Morphological Image Processing
Metallic Foams
Low-Level Programming

LANGUAGES

English (bilingual)
Polish (bilingual)
German (intermediate (3y))
French (intermediate (3y))
Croatian (basic)

NON-ACADEMIC INTERESTS

- Large Format Photography
- Camera and Lens Design
- Sailing (4000+h experience)
- Paragliding (2016-Now)
- Cycling Hundreds of Miles
- Sailboat Design
- Coffee Preparation
- Good Movies
- Affordable Traveling

I've had the pleasure of visiting: Albania, Antigua, Aruba, Austria, Belgium, Bosnia, Bulgaria, Canada, Croatia, Czech Republic, Denmark, Dominica, Egypt, England, Estonia, Finland, France, Germany, Greece, Grenada, Hungary, Iceland, Ireland, Italy, Latvia, Liechtenstein, Lithuania, Luxembourg, Macedonia, Morocco, Monaco, Montenegro, Montserrat, Netherlands, Norway, Isle of Man, Oman, Poland, Portugal, Qatar, Romania, Saint Lucia, Saint Vincent, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Thailand, Turkey, Turks and Caicos, United Arab Emirates, United Kingdom, Vatican, Vietnam, and **39 US States**

SELECTED PAST RESEARCH

Advisor: Prof. Matthew A. Willard December 2015 — December 2019
Case Western Reserve University

B.S. Thesis 08/2018 – 12/2019
Computational Design of Iron-based Amorphous Alloys for Near-Room-Temperature Magnetocaloric Refrigeration

Leading Researcher 10/2016 – 12/2018
Indirect Measurement of Wetting Propagation of Resins in Porous Catalyzing Medium System (with Hidden Markov Chain Modeling)

Pet Project 03/2016 – 09/2019
Development of Methods for Printing of Anodic Oxide Layer Maps on Titanium

Project Group Leader for St. Gobain Design Competition 12/2015 – 05/2016
CeramSalt Project for Development of Ceramic–Salt Matrix Deicing Material

Advisor: Prof. Gerhard E. Welsch September 2015 – October 2016
Case Western Reserve University

Leading Researcher 01/2016 – 10/2016
Cyclic Electrochemical Treatment of Titanium Alloys for Oxide Layer Topology Modifications

Undergraduate Researcher 09/2015 – 05/2016
Ti-Zr Alloy Based Electrochemical Capacitors

Selected Personal Projects May 2013 – Present
CWRU / PSU

PSU Course & Personal 09/2021 – Present
Additive Manufacturing of Camera Lenses using Stereolithography

CWRU **B.E. Engineering Capstone** 01/2019 – 06/2019
Design and Testing of a Thumb Prosthetic

Sole Researcher 01/2018 – 05/2019
Changes in the Conductivity of FDM-Printed Graphene-Infused PLA under Electrical Stress

Sole Researcher 10/2017 – Present
Development of 4 and Higher-Dimensional Dataset Visualization Methods for HEAs

PROFESSIONAL ORGANIZATIONS

ASM (2016-Now) **TMS** (2016-Now) **MRS** (2017-Now)
MaRDA (2023-Now) **CECAM** (2023-Now) **ACerS** (2016-Now)
IEEE (2017-2021) **MGF** (2019-Now) **NSF ERVA** (2022-Now)

BIOGRAPHICAL NOTE

I was born in Europe, where I spent my childhood and received pre-college education. The public school I attended was nationally recognized for its university-level chemistry curriculum, and my triple major in Physics, Chemistry, and Biology quickly propelled me toward seeking an advanced degree in physical sciences, eager to make my mark.

I first came to the United States in 2013 and moved entirely in 2015 when I joined the Materials Science Department at Case Western Reserve University. Within the first two months of enrollment, I began research in Prof. Welsch's group, and after my first year, I started to take graduate courses. Around the same time, I joined Prof. Willard's group, progressively moving from experiments towards theory, modeling, and simulations. In late 2016, this led me to enroll in graduate courses in Artificial Intelligence and specialize in applying Machine Learning to problems in Materials Science.

I earned my BSE degree in 2019 and moved directly to pursue my PhD at Penn State under world-renowned thermodynamics expert Prof. Zi-Kui Liu. Now, I have the pleasure of working on implementing a variety of computational techniques, including machine learning, while having the support of colleagues who are specialists in ab-initio modeling, thermodynamic calculations, and materials discovery. Since 2022, I also extensively collaborate with LLNL and have spent two summers on-site at the lab.

PUBLICATIONS

Google Scholar | **ORCID** | **Scopus** | **Software** |

- W. Li, L. Raman, A. Debnath, *et al.*, "Design and validation of refractory alloys using machine learning, CALPHAD, and experiments," *International Journal of Refractory Metals and Hard Materials*, vol. 121, p. 106 673, Jun. 2024. DOI: 10.1016/j.ijrmhm.2024.106673
- A. Debnath, L. Raman, W. Li, *et al.*, "Comparing forward and inverse design paradigms: A case study on refractory high-entropy alloys," *Journal of Materials Research*, vol. 38, no. 17, pp. 4107–4117, Sep. 2023. DOI: 10.1557/s43578-023-01122-6
- A. M. Krajewski, J. W. Siegel, J. Xu, *et al.*, "Extensible Structure-Informed Prediction of Formation Energy with improved accuracy and usability employing neural networks," *Computational Materials Science*, vol. 208, p. 111 254, Jun. 2022. DOI: 10.1016/j.commatsci.2022.111254
- S. Im, S. L. Shang, N. D. Smith, *et al.*, "Thermodynamic properties of the Nd-Bi system via emf measurements, DFT calculations, machine learning, and CALPHAD modeling," *Acta Materialia*, vol. 223, p. 117 448, Jan. 2022. DOI: 10.1016/J.ACTAMAT.2021.117448
- A. Debnath, A. M. Krajewski, H. Sun, *et al.*, "Generative deep learning as a tool for inverse design of high entropy refractory alloys," *Journal of Materials Informatics*, vol. 1, no. 1, p. 3, Sep. 2021. DOI: 10.20517/jmi.2021.05
- S.-L. Shang, H. Sun, B. Pan, *et al.*, "Forming mechanism of equilibrium and non-equilibrium metallurgical phases in dissimilar aluminum/steel (Al–Fe) joints," *Scientific Reports*, vol. 11, no. 1, p. 24 251, Dec. 2021. DOI: 10.1038/s41598-021-03578-0
- X. Chong, S. L. Shang, A. M. Krajewski, *et al.*, "Correlation analysis of materials properties by machine learning: illustrated with stacking fault energy from first-principles calculations in dilute fcc-based alloys," *Journal of Physics: Condensed Matter*, vol. 33, no. 29, p. 295 702, Jun. 2021. DOI: 10.1088/1361-648X/AC0195

UNDER REVIEW

- A. M. Krajewski, J. W. Siegel, and Z.-K. Liu, "Efficient Structure-Informed Featurization and Property Prediction of Ordered, Dilute, and Random Atomic Structures," Apr. 2024
- A. M. Krajewski, A. M. Beese, W. F. Reinhart, *et al.*, "Efficient Generation of Grids and Traversal Graphs in Compositional Spaces towards Exploration and Path Planning Exemplified in Materials," Feb. 2024. DOI: 10.48550/arXiv.2402.03528
- A. M. Krajewski, A. Debnath, W. F. Reinhart, *et al.*, "nimCSO: A Nim package for Compositional Space Optimization," Mar. 2024. DOI: 10.48550/arXiv.2403.02340
- M. L. Evans, J. Bergsma, A. Merkys, *et al.*, "Developments and applications of the OPTIMADE API for materials discovery, design, and data exchange," Feb. 2024. DOI: 10.48550/arXiv.2402.00572
- H. Sun, B. Pan, Z. Yang, *et al.*, "MaterialsMap: A CALPHAD-Based Tool to Design Composition Pathways through feasibility map for Desired Dissimilar Materials, demonstrated with RSW Joining of Ag-Al-Cu," Mar. 2024

IN-PREPARATION

1. Adam M. Krajewski, Jonathan Siegel, Ricardo Amaral, Zi-Kui Liu *"crystALL Toolkit for Pure Data Driven Structure Prediction"* (to be submitted to JOSS in March 2024)
2. Lavanya Raman, Arindam Debnath, Shuang Lin, Erik Furton, Adam Krajewski, Marcia Ahn, Shunli Shang, Shashank Priya, Zi-Kui Liu, Allison M. Beese, Wesley Reinhart, Wenjie Li *"Microstructure and mechanical properties of Mo-Nb-Ti-V-W-Zr refractory multi-component alloys developed using a data-driven inverse design approach"* (April 2024)

3. Adam M. Krajewski, Jonathan Siegel, Ricardo Amaral, Zi-Kui Liu *"MPDD: Material-Property-Descriptor Database"* (to be submitted to Computational Materials Science in April 2024)

4. Adam M. Krajewski, Arindam Debnath, Wesley Reinhart, Zi-Kui Liu *"Composition Design Space Optimization for High Entropy Alloys"* (to be submitted to Computational Materials Science in Spring 2024)

5. Adam M. Krajewski, Brandon Bocklund, Kate Elder, Joseph T. McKeown, Aurelien Perron *"High-Throughput Physics-Informed Exploration of Compositionally Complex Design Space for Targeted Properties and Structure"* (to be submitted to Nature Computational Science in June 2024)

6. Adam M. Krajewski, Arindam Debnath, Shuang Lin, Hui Sun, Wesley Reinhart, Allison Beese, Zi-Kui Liu *"ULtrahigh TEmperature Refractory Alloys (ULTERA) Database"* (to be submitted to npj Computational Materials in July 2024)

7. Kate Elder, Adam M. Krajewski, Brandon Bocklund, Zi-Kui Liu, Joseph T. McKeown, Aurelien Perron *"Ductility Modelling of Refractory High Entropy Alloys"* (Fall 2024)

8. Adam M. Krajewski, Zi-Kui Liu *"CSN 1.0: Compact Structure Notation for Storing Billions of Crystal Structures"* (Fall 2024)