KHALED HIRMAS, PhD

Materials Science & Engineering

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PROFESSIONAL PROFILE

Materials Scientist and Engineer with a PhD in Materials Science & Engineering and extensive academic, research, teaching, and industrial experience spanning computational materials science, experimental materials characterization, metallurgy, semiconductor materials, solid-state physics, mechanical engineering, and data science/machine learning. Experienced university educator with teaching experience at the University of Texas at Arlington and the University of Tripoli, including Introduction to Materials Science, Solid-State Physics, Solid-State Electronic Devices, Thermodynamics of Materials, Physical Metallurgy, Corrosion, Non-Destructive Testing, Failure Analysis, and Transport Phenomena. Research expertise includes Density Functional Theory (DFT), molecular dynamics (MD), Monte Carlo methods, materials thermodynamics, phase stability, phonon calculations, defects, surfaces, electronic structure, mechanical properties, and high-performance computing. Doctoral research focused on the copper-rich side of the Al–Cu phase diagram, including intermetallic phases, thermodynamic stability, phonons, electronic structure, and mechanical properties. Strong experimental background in metallography, fractography, XRD, SEM/EDX, AFM/STM, XPS, Raman/FTIR, mechanical testing, corrosion testing, microhardness, and NDT. Completed a Data Science and Machine Learning Certificate from the University of Toronto and a Semiconductor Fabrication & Inspection Micro-Credential, with interest in applying data-driven methods to accelerate materials discovery, predict materials properties, identify structure–property relationships, optimize processing conditions, and integrate computational predictions with experimental research.

RESEARCH INTERESTS

- Computational Materials Science; Materials Informatics and Machine Learning for Materials Discovery
- Density Functional Theory (DFT), Molecular Dynamics (MD), Materials Thermodynamics and Phase Stability
- Semiconductor Materials, Fabrication and Characterization; Thin Films and Surface Science
- Nanomaterials, 2D Materials and Graphene; Magnetic and Electronic Materials
- Shape-Memory Alloys and Functional Materials; Solid-State Synthesis and Materials Processing
- Materials Characterization, Fracture Mechanics and Mechanical Behavior
- Computational–Experimental Integration

EDUCATION

PhD, Materials Science & Engineering

University of Texas at Arlington, USA | 2012–2018 | GPA: 4.00/4.00

Dissertation: Computational Study on the Copper-Rich Side of the Aluminum–Copper Phase Diagram. Research included first-principles calculations, molecular dynamics, thermodynamics, phase stability, intermetallic structures, phonons, defects, surfaces, electronic properties, and mechanical properties.

MEng, Materials Science & Engineering

University of Texas at Arlington, USA | 2012–2016 | GPA: 4.00/4.00

MSc, Materials Science & Engineering

Christian-Albrechts-Universität zu Kiel, Germany | 2003–2007

Research and laboratory training in materials testing, functional materials, surface science, nanostructuring, and scientific methods.

BSc, Materials Science & Metallurgical Engineering

University of Tripoli, Libya | 1987–1992

Diploma, Mechanical Design & Technology

Metro College of Technology | 2026 | With Distinction

Training in AutoCAD, SolidWorks, Autodesk Inventor, CATIA, ANSYS FEA/CFD, GD&T, engineering drawing, mechanical design, and simulation.

CERTIFICATIONS & PROFESSIONAL TRAINING

- Data Science and Machine Learning Certificate — University of Toronto, Data Sciences Institute | 2024
- Semiconductor Fabrication & Inspection Micro-Credential — University of Toronto, MSE & ECE | 2025
- Materials Testing Laboratory Certificate — Christian-Albrechts-Universität zu Kiel, Germany
- Functional Materials Laboratory Certificate — Christian-Albrechts-Universität zu Kiel, Germany
- Scientific Methods Laboratory Certificate — Christian-Albrechts-Universität zu Kiel, Germany

RELEVANT EXPERIENCE

PhD Researcher – Computational Materials Science

University of Texas at Arlington, USA

- Conducted first-principles DFT calculations using Quantum ESPRESSO and molecular dynamics simulations using LAMMPS to investigate Al–Cu alloys.
- Investigated electronic structure, crystal structures, phase stability, thermodynamics, phonons, defects, surface energies, and mechanical properties.
- Developed Python and Bash workflows for automated and high-throughput computational materials research.
- Performed multi-node simulations on HPC clusters and managed large computational datasets and thousands of simulation jobs.
- Calculated phonon band structures, elastic constants, electronic properties, defect energies, and surface energies.
- Investigated Cu_3Al $L1_2$ and $D0_{22}$ structures and their thermodynamic and mechanical stability.
- Collaborated with experimental researchers to compare computational predictions with experimental observations.

Teaching Assistant – Materials Science and Engineering

University of Texas at Arlington, USA

- Contributed to teaching undergraduate courses in Introduction to Materials Science, Solid-State Physics, and Solid-State Electronic Devices.
- Assisted faculty with lectures, tutorials, laboratory activities, assignments, examinations, and student assessment.
- Provided individual and group instruction and connected fundamental materials science concepts with engineering applications.
- Assisted in developing course materials, problem sets, laboratory exercises, and instructional content.

Assistant Lecturer – Materials Science and Engineering

University of Tripoli, Libya

- Taught undergraduate engineering courses in Materials Science, Thermodynamics of Materials, and Solid-State Physics.
- Delivered lectures covering crystal structures, phase transformations, thermodynamics, diffusion, solid-state properties, and materials behavior.
- Developed course materials, laboratory exercises, assignments, and assessments.
- Guided students in understanding theoretical concepts and their applications to engineering materials.

Teaching Assistant – Materials Science and Metallurgical Engineering

University of Tripoli, Libya

- Supported undergraduate teaching and laboratory activities in Materials Science, Physical Metallurgy, Corrosion and Corrosion Control, Solid-State Physics, Transport Phenomena, NDT, Failure Analysis, and Thermodynamics of Materials.

Metallurgical Engineer

Libyan Iron and Steel Company – Misrata, Libya

- Prepared and analyzed metallographic samples using grinding, polishing, and etching techniques.
- Conducted qualitative and quantitative metallurgical analysis of ferrous alloys.
- Conducted materials investigations using stereomicroscopy, optical microscopy, SEM, and EDX.
- Performed microhardness testing, NDT, and corrosion testing and prepared technical reports.

RESEARCH EXPERIENCE & PROJECTS

Computational Study of the Copper-Rich Side of the Aluminum–Copper System

PhD Dissertation – University of Texas at Arlington | 2016–2018

- Applied DFT and molecular dynamics to investigate the structure and stability of Al–Cu alloys.
- Used Quantum ESPRESSO for ab initio calculations and LAMMPS for molecular dynamics.
- Investigated phase stability, phase separation, intermetallic structures, and thermodynamic properties.
- Calculated phonon band structures, elastic constants, mechanical properties, and electronic properties.
- Developed Python/Bash workflows for high-throughput computational studies and utilized HPC resources.

Machine Learning and Data Science Project: Predicting Heart Disease

University of Toronto – Data Sciences Institute | 2024

- Developed machine-learning models using Python, scikit-learn, and TensorFlow, including KNN, Logistic Regression, Random Forest, and Neural Networks.
- Performed data preprocessing, feature engineering, dimensionality reduction, model evaluation, and hyperparameter optimization.
- Achieved over 92% predictive accuracy using cross-validation and model optimization.
- Developed transferable skills for materials-property prediction, materials screening, process optimization, and accelerated materials discovery.

Solid-State Electrochemical Oxygen Pump

University of Düsseldorf, Germany | January–August 2006

- Designed and successfully fabricated a solid-state electrochemical oxygen pump for ultra-high-vacuum applications.
- Investigated oxygen interactions with surface point defects on TiO_2 (110) using in-situ scanning tunneling microscopy.
- Obtained atomic-resolution images of prepared surfaces and demonstrated successful operation under UHV conditions.

EXPERIMENTAL & CHARACTERIZATION EXPERIENCE

- Materials Characterization: XRD, SEM/EDX, AFM, STM, XPS, Raman, FTIR, UV–VIS, VSM, DMA
- Metallurgy & Testing: Metallography, optical microscopy, fractography, microhardness, mechanical testing, fracture mechanics, corrosion testing, NDT
- Materials Science: Phase transformations, deformation and recrystallization, precipitation and diffusion, thermal analysis
- Functional & Advanced Materials: Shape-memory alloys, porous silicon, surface functionalization, surface nanostructuring, thin films, electrochemical materials, solar-cell characterization

COMPUTATIONAL & ENGINEERING SKILLS

- Computational Materials: DFT, Quantum ESPRESSO, MD, LAMMPS, Monte Carlo, phonons, defects/surfaces, thermodynamics, phase stability, electronic structure, HPC
- Data Science & ML: Python, TensorFlow, scikit-learn, Pandas, NumPy, Matplotlib, Seaborn, statistical analysis, predictive modeling, deep learning
- CAD/FEA: ANSYS FEA/CFD, SolidWorks, Autodesk Inventor, AutoCAD, CATIA, GD&T / ASME Y14.5, tolerance analysis, engineering drawing
- Programming & Computing: Python, MATLAB, SQL, Bash, Git/GitHub, Linux/Unix, Windows, workflow automation

SELECTED PUBLICATIONS & PATENTS

- Anti-Lotus Effect for Nanostructuring at the Leidenfrost Temperature, Advanced Materials, 2007. Featured as inside front cover.
- Metallurgical Investigation on Reboiler Tube Failure, Engineering Research Journal, Libya, 1997.
- Formation of Cu_3Al-$D0_{22}$ Order Phase in Al–Cu Diffusion Interface at Temperature Beyond Equilibrium Limit, Materials Chemistry and Physics — manuscript under review.
- First-Principles Calculation of Structural, Thermodynamic, Elastic, and Electronic Properties of Cu_3Al $L1_2$ and $D0_{22}$ Structures and Superstructures — manuscript in preparation.
- German Patent: DE102007053157(A1), 2009.
- Dissertation: Computational Study on the Cu-Rich Side of Aluminum–Copper Phase Diagram, University of Texas at Arlington, 2018.

AWARDS, FELLOWSHIPS & SCHOLARSHIPS

- Graduate Studies Dissertation Fellowship — University of Texas at Arlington | 2018
- Academic Excellence Award — University of Texas at Arlington | 2013–2018
- Materials Science & Engineering Scholarship — University of Texas at Arlington | 2017
- Kelcy Warren Graduate Engineering Fellowship — University of Texas at Arlington | 2016
- Graduate School General Fellowship — University of Texas at Arlington | 2013, 2014, 2015
- Golden Key International Honour Society — University of Texas at Arlington | 2014
- Libyan Ministry of Education Scholarship — PhD | 2011
- Libyan Ministry of Education Scholarship — MSc | 2003

ACADEMIC & RESEARCH INTERESTS

- Materials discovery using machine learning and computational materials science
- DFT and molecular dynamics of advanced materials
- Semiconductor materials, fabrication, and characterization
- 2D materials, graphene, and nanostructured materials
- Magnetic and electronic materials
- Shape-memory alloys and functional materials
- Solid-state synthesis and materials processing
- Thermodynamics and phase stability of alloys and intermetallic compounds
- Materials fracture, corrosion, and mechanical behavior
- Integration of computational predictions with experimental materials characterization

LANGUAGES

Tamazight — Native | Arabic — Native | English — Professional/Academic | German — Academic/Professional background