

Ridwan Sakidja

Professor, Matthew & Patricia Harthcock CNAS Faculty Fellow, Director of Materials Science Program

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Education:

- PhD. Metallurgy (August 2003), University of Wisconsin-Madison
- B.S. Metallurgical Engineering with Materials Science Option (December 1993) University of Wisconsin-Madison

Work Experience:

Professor

Department of Physics, Astronomy, and Materials Science, Missouri State University

August 2019 – Present

- Teach undergraduate and graduate-level courses in Physics and Materials Science, including:
 - MAT792: Computational Materials Science
 - MAT790: Statistical Applications on Materials Science
 - MAT720: Advanced Quantum Mechanics
 - MAT580/681: Structure of Solids
 - MAT514/614: Techniques in Electron Microscopy
 - MAT509/609: Advanced Computational Methods in Science
 - MAT540/640: Thermodynamics of Materials
 - PHY575/675: Quantum Mechanics
 - PHY509/609: Special Topics in Physics and Astronomy
 - Neural Networks and Machine Learning
 - Introduction to Quantum Computing (with Xanadu, a PennyLane developer)
 - PHY486: Undergraduate Research II
 - PHY386: Undergraduate Research I
 - PHY353: Electricity and Magnetism
 - PHY319: Mathematics for Science and Engineering I
 - PHY291: Introduction to Computational Physics
 - PHY203: Foundations of Physics I
 - PHY123: Introduction to Physics I
- Conduct computational materials physics research on structural and functional applications of high-temperature alloys, nanomaterials, hybrid nanostructures, drug discoveries, and nuclear materials using supercomputer facilities at NERSC, TACC, and GPU workstations at MSU.

Associate Professor

Department of Physics, Astronomy, and Materials Science, Missouri State University

August 2014 – August 2019

Associate Research Professor

Department of Physics and Astronomy, University of Missouri-Kansas City (UMKC)

January 2013 – August 2014

- Conducted computational materials research on the mechanical properties and environmental resistance of structural intermetallics and non-crystalline materials.
- Developed new computational methods to generate a high-throughput materials database for structural intermetallics and complex structures.
- Supervised graduate students and postdoctoral fellows in the Electronic Structure Group (PI: Prof. W-Y Ching) on ab initio molecular dynamics (AIMD)-related materials research.

Associate Lecturer

Department of Materials Science & Engineering, University of Wisconsin-Madison (UW-Madison)
Fall 2011 & Fall 2012

- Taught MSE330: Thermodynamics of Materials, a 4-credit undergraduate core course.

Assistant Scientist

Department of Materials Science & Engineering, University of Wisconsin-Madison (UW-Madison)
October 2006 – December 2012

- Conducted research and development in high-temperature coating materials for structural applications with external and internal funding support:
 - NSF Grant: Design and synthesis of low-temperature corrosion-resistant aluminide coatings for advanced Cr steels. Role: Co-Principal Investigator.
 - ONR Grant: Multilayer Coatings for Enhanced Oxidation Resistance in High-Temperature Mo-Si-B Alloys. Role: Senior Research Personnel.
 - Draper Technology Innovation Fund (TIF) Grant: Enhanced Applications of Borosilica Coatings for Ultra-high Temperature Materials. Role: Co-Principal Investigator.
 - Johnson Control's Grant: Materials Characterization and Molecular Modeling Examination of Impact of Metal Contaminants on the Performance of Li-Ion Batteries. Role: Co-Principal Investigator.
 - AFOSR Grant: Phase Stability and Multiphase Designs in High Temperature Refractory Metal-Si-B Alloys. Role: Senior Research Personnel.
 - DOE/NETL Grant: Multi-Scale Computational Design and Synthesis of Protective Smart Coatings for Refractory Metal Alloys. Role: Senior Research Personnel.
 - DOE/NEUP Grant: Modeling Solute Thermokinetics in LiCl-KCl Molten Salt for Nuclear Waste Separation. Role: Research Staff.

Research Associate

Department of Materials Science & Engineering, University of Wisconsin-Madison (UW-Madison)
September 2003 – October 2006

- Conducted research and development in high-temperature oxidation-resistant alloys and coatings for structural applications with support from AFOSR and ONR agencies:
 - Assessed high-temperature phase equilibria and defect structures in Mo-Si-B ternary system (AFOSR).
 - Conducted computational alloying design in Mo-based borosilicide phase (AFOSR).
 - Synthesized multi-layer Mo-Si-B coating structures into Mo-Si-B alloys with integrated diffusion barriers (ONR).

Research Assistant

Department of Materials Science & Engineering, University of Wisconsin-Madison (UW-Madison)
March 1996 – September 2003

- Developed alloying design for high-temperature Mo-Si-B alloys.
- Analyzed phase stability of complex Mo-based silicides and borosilicides.
- Synthesized rapidly quenched Mo-Si-B metallic glass and in-situ nanocomposite.

Research Staff

Nuclear Atomic Energy Agency of Indonesia (BATAN), Department of Nuclear Metallurgy
January 1994 – December 1995

- Investigated oxidation resistance of zirconium-based alloys.
- Assisted technicians in the use of powder sintering and heat-treatment equipment.

Undergraduate Researcher

Department of Materials Science & Engineering, University of Wisconsin-Madison (UW-Madison)
July 1991 – December 1993

- Assisted in the development of computer simulation of fluid flow in silicone oil floating zone.
- Investigated Hall-Petch relationship in W/Cu multi-layer ultra-thin film.
 - Investigated melting reactions in Bi-Sr-Ca-Cu (2212) oxides.

Awards and Honors:

Secured a total of \$3M in collaborations with research institutions, National Laboratories, and industries

- **Airbus and BMW Quantum Computing Challenge 2024:** The Quantum Mobility Quest, with a project titled "Scalable Oxidation Modeling of Aluminum Surface using Quantum Computing". (June - December 2024). [Leads MSU team as top 3 finalists for "Smart Coatings" category. Other teams: USC and InhibitQ.](#)
- **DOE Visiting Faculty Program Fellowship,** Lawrence Berkeley National Laboratory (LBNL), Summer 2024: AI-enabled Computational Materials Science to Model Degradation in Molten Salt Reactor (MSR). Host: Mark Asta. (June - August 2024)
- **Quantum Information Science QIS@Perlmutter Award:** Computational Project, "Quantum Precision: ALD-Driven Modeling for Superconducting Qubit Fabrication". (March 2024 – January 2025)
- **NASA-Missouri Space Grant Consortium Affiliates Award:** Development of efficient machine learning interatomic potentials to model critical structural materials for interplanetary missions. (October 2023 – July 2024)
- **Endowed Dr. Matthew & Patricia Harthcock CNAS Faculty Fellow.** (2023-2026)
- **DOE Visiting Faculty Program Fellowship,** Lawrence Berkeley National Laboratory (LBNL), Summer 2022. Host: Kristin Persson. (June - August 2022)
- **Principal Investigator, NERSC-supported Supercomputer Project** (DOE-BES-Materials Sciences and Engineering): Phase Stability in High-melting and Corrosion Resistant Borosilicidates, Aluminides, and Novel Carbides at Perlmutter Supercomputer Clusters. (2022)
- **DOE Visiting Faculty Program Fellowship,** Lawrence Berkeley National Laboratory (LBNL), Summer 2021 (Virtual). Host: Kristin Persson. (June - August 2021)
- **Co-Principal Investigator, NASA-Missouri Space Grant Consortium Affiliates Award: AIDE:** Artificial Intelligence for Defect Examination, PI: Sheryl Brahmam. (2020-2021)
- **Outstanding Thesis Advisor Award,** Graduate College, Missouri State University. (2020)
- **Co-Principal Investigator, NSF Grant No. 1902069** (Advanced Manufacturing Program): Composition-Microstructure-Property Relationships in Entropy-Stabilized Boride Ceramics, in collaboration with Missouri University of Science & Technology. (September 2019 - August 2022)
- **Principal Investigator, NSF Grant No. 1809284** (Electronics, Photonics, and Magnetic Devices Program): Collaborative Research on Development of Atomically Thin Tunnel Barriers for High-Performance Tunnel Junctions, at Missouri State in collaboration with KU. (September 2018 - August 2022)
- **Principal Investigator, NETL-DOE Grant No. FE0031554** (Crosscutting Research Program): Multimodal Approach to Modeling Creep Deformation in Ni-base Superalloys at Missouri State in collaboration with UMKC and Missouri S&T. (December 2017 - March 2022)
- **Principal Investigator, NSF Grant No. 1729176** (Designing Materials to Revolutionize and Engineer our Future Program): Collaborative Research on Predictive Modeling of Polymer-Derived Ceramics, in collaboration with UMKC and Ohio State. (October 2017 - September 2021)
- **Principal Investigator, Google Cloud Platform Project: ICME2:** Informatics Consortium for Materials under Extreme Environments. (2019-2020)
- **Co-Principal Investigator, Curriculum Innovation Project:** Impact Cratering: Physics and Geology of Craters and Impact Structures, Missouri State University. (2018-2019)
- **Faculty Excellence in Research Award,** College of Natural and Applied Sciences (CNAS), Missouri State University. (2019)
- **Co-Principal Investigator, NSF-supported XSEDE Supercomputer Project (DMR160177):** DFT-Based Calculations of Concentration-Dependent and Finite-Sized Effects in New Classes of Bimagnetic Core-Shell Nanoparticles, PI: Robert Mayanovic. (2018-2019)
- **Principal Investigator, NSF-supported XSEDE Supercomputer Project (DMR180012):** Ab-Initio Molecular Dynamics Study on the Ionic Mobility in Li-Ion Based Solid-State Electrolytes, Co-PI: S. Mitra. (2018-2019)
- **Missouri State University Foundation Award for Excellence in Research.** (2018)

- **Principal Investigator, NASA-Missouri Space Grant Consortium Affiliates Award:** Hands-On Virtual Reality (VR) Applications to Investigate Mechanical and Chemical Integrity of Carbon-Based Nanocomposites, Co-PI: Razib Iqbal. (2017-2018)
- **Co-Principal Investigator, NSF-supported XSEDE Supercomputer Project (DMR160177):** First Principles Calculations of Novel Structural Phases in Bimagnetic Core-Shell Nanoparticles, PI: Robert Mayanovic. (2017-2018)
- **Co-Principal Investigator, Curriculum Innovation Project:** Cross-curricular Biophysics Laboratory Experiences, Missouri State University. (2017-2018)
- **Co-Principal Investigator, NorthStar Battery Research Contracts:** Minimizing Sn Segregation during PbSn Rolling Process & Water Loss through Polymer-Based Lead-Acid Battery Casings, PI: R. Mayanovic. (2017)
- **Co-Principal Investigator, Curriculum Innovation Project:** Immersive Virtual Reality (VR) Technologies for Introductory Physics Education, PI: R. A. Baker, Co-PI: Amir H. Behzadan, Missouri State University. (2016-2017)
- **Principal Investigator, NASA-Missouri Space Grant Consortium Affiliates Award:** Multi-scale Design in Multi-functional Carbon-Based Nanocomposites. (2016-2017)
- **Missouri State University Summer Faculty Fellowship Award:** Design and Synthesis of Oxidation and Corrosion Resistant Protective Coatings. (2016)
- **Principal Investigator, DOE's NERSC-supported Supercomputer Project:** Phase Stability in High-melting and Corrosion Resistant Borosilicides. (2012-2015)
- **Co-Principal Investigator, NSF Grant No. 0926796:** The Design and Analysis of Aluminide Surface Layers for Low-temperature Synthesis, PI: Prof. J.H. Perepezko. (September 2009 - July 2012)
- **Co-Principal Investigator, Johnson Control's Advancements in Battery Energy Storage Systems Grant:** Materials Characterization & Molecular Modeling Examination of Impact of Metal Contaminants on the Performance of Li-Ion Batteries, PI: Ben Church, UWM & J. H. Perepezko, UW-Madison. (2012)
- **Co-Principal Investigator, Draper Technology Innovation Fund (TIF) Grant:** Enhanced Applications of Borosilica Coatings for Ultra-high Temperature Materials, PI: Prof. J.H. Perepezko. (July 2011 - June 2012)

Professional Societies and Services:

- Members of American Physics Society (APS) and American Ceramic Society (ACerS).
- Materials Science Graduate Program Director, Missouri State University (2023-Present).
- Graduate Council (PAMS Dept. Representative), Missouri State University (2019- 2020), (2023-Present).
- Member of Inclusive Engagement Council of Missouri State University (2024 -Present)
- Master of Natural and Applied Science (MNAS) Interdisciplinary Graduate Program Coordinator for PAMS Dept., Missouri State University (2017-2019), (2022-Present).
- Personnel Committee Chair, PAMS Dept., Missouri State University (2021-Present).
- CNAS Diversity, Equity, and Inclusion (DEI) Committee Member, Missouri State University (2020 - Present).
- Reviewer for *Acta Materialia*, *Advanced Materials*, *ChemEngineering*, *Crystals*, *Intermetallics*, *J. Alloys & Compounds*, *J. Nuclear Materials*, *Metallurgical Transactions A and B*, *Oxidation of Metals*, *Scientific Reports*, *Scripta Materialia*, and *Surface & Coating Technology*.
- Lead Organizer of Symposium on Synergy in Multi-scale Modeling and Experiments to Resolve Complex Disordered Solids held at the 2018 Materials Science & Technology (MS&T) in Columbus, OH (October 14-18, 2018).
- Faculty Senate (PAMS Dept. Representative), Missouri State University (2017-2019).
- Acting Graduate Coordinator of the Materials Science Graduate Program in PAMS Dept., Missouri State University (Fall 2017).
- Topical Editor of *Journal of Metals (JOM)* for Refractory Metals and Alloys (2012- 2014).

- Lead Organizer of Symposium on Beyond Nickel Base Superalloys II at the Materials Science & Technology Conference & Exhibition (MS&T- 2012) held in Pittsburgh, Pennsylvania (October 7- 11, 2012).
- Lead Organizer of Symposium on Advanced Protective Coatings for Refractory Metals and Alloys at the Materials Science & Technology Conference & Exhibition (MS&T-2011) held in Columbus, OH. (Oct.16-20, 2011).

Journal Publications:

1. A. A. Odusanya, D. Kumar, J. D. Schall, J. Mayer, R. Sakidja, "Computational approach to modeling electronic properties of titanium oxynitride systems", *Computational Materials Science*, 245, 113292, (2024).
2. S. San, P. Adhikari, R. Sakidja, J. Brechtel, P. K. Liaw, and W-Y Ching, "Porosity modeling in a TiNbTaZrMo high-entropy alloy for biomedical applications", *RSC Advances*, 13, 36468-36476 (2023).
3. A. I. Duff, R. Sakidja, H.C. Walker, R. A. Ewings and D. Voneshen, "Automated potential development workflow: Application to BaZrO₃", *Computer Physics Communications*, 108896, 293 (2023).
4. Wai-Yim Ching, Saro San, Caizhi Zhou and Ridwan Sakidja, "Ab Initio Simulation of Structure and Properties in Ni-Based Superalloys: Haynes282 and Inconel740", *Materials*, 16[2], 887 (2023).
5. A. Tanji, R. Feng, Z. Lyu, R. Sakidja, P. K. Liaw, H. Hermawan, "Passivity and corrosion resistance of Al₂₀Cr₅Fe₅₀Mn₂₀Ti₅ and Al₇Cr_{23.26}Fe_{23.26}Co_{23.26}Ni_{23.26} high-entropy alloys in Hanks' solution", *Corrosion Science*, 210, 110828 (2023).
6. A. Tanji, X. Fan, R. Sakidja, P. K. Liaw, and H. Hermawan, "Niobium addition improves the corrosion resistance of TiHfZrNbx high-entropy alloys in Hanks' solution", *Electrochimica Acta*, 424, 140651 (2022).
7. T. McGilvry-James, B. Timalina, M. M. Mou, and R. Sakidja, "Deep potential development of transition-metal-rich carbides", *MRS Advances*, 7, pp. 468–473 (2022).
8. D. Romine and R. Sakidja, "Modeling atomic layer deposition of alumina using reactive force field molecular dynamics", *MRS Advances*, 7, 185-189 (2022).
9. WC Yang, S Lee, CH Chung, R Sakidja, JS Park, "Ablation Stability of In Situ Al₂O₃ Layer in Aluminized AISI 4130 Steels under High-Temperature Plasma Flame Environments" *Journal of Materials Engineering and Performance*, 30, 7488–7493, (2021).
10. K. Baral, S. San, R. Sakidja, A. Couet, K. Sridharan, and W-Y Ching, "Temperature-Dependent Properties of Molten Li₂BeF₄ Salt Using Ab Initio Molecular Dynamics", *ACS Omega*, 6[30], 19822–19835, (2021).
11. M. Gong, B. Timalina, R. Sakidja, J. T. Douglas, J. Z. Wu, "Ligands Anchoring Stabilizes Metal Halide Perovskite Nanocrystals", *Advanced Optical Materials*, 9, 2101012 (2021).
12. R. Goul, A. Marshall, R. Sakidja and J. Wu, "Investigation of in-vacuo atomic layer deposition of ultrathin MgAl₂O₄ using scanning tunneling spectroscopy", *ACS Applied Electronic Materials*, 2[10], 3121-3130 (2020).
13. M. Abbasi, S. Im, J. Johnson, G. Ortiz, M. Zhu, N. Oyler, M. Paquette, P. Rulis, R. Sakidja, J. Hwang, "Direct Determination of Medium Range Ordering in Amorphous Hydrogenated Boron Carbide for Low-k Dielectric Applications", *Microscopy and Microanalysis*. 26[S2], pp. 248 – 249 (2020).
14. W-Y Ching, S. San, J. Brechtel, R. Sakidja, M. Zhang, and P. Liaw, "Fundamental electronic structure and multiatomic bonding in thirteen biocompatible high-entropy alloys", *npj Computational Materials*, 6[45] (2020).
15. N. Baishnab, R. Khadka, M. Paquette, P. Rulis, N. Oyler, J. Hwang, R. Sakidja, "Role of Generated Free Radicals in Synthesis of Amorphous Hydrogenated Boron Carbide from ortho-Carborane using Argon Bombardment: A ReaxFF Molecular Dynamics Study", *Materials Research Express*, 6[12], 126461 (2020).
16. S. Ghopry, M. Alamri, R. Goul, B. Cook, S. Sadeghi, R. Gutha, R. Sakidja, J. Z. Wu, "Au Nanoparticles/WS₂ Nanodomains/Graphene van der Waals Heterostructure Substrates for Surface-Enhanced Raman Spectroscopy", *ACS Applied Nano Materials*, 3[3], 2354-2363 (2020).

17. R. Khadka, N. Baishnab, G. Opletal and R. Sakidja, "Study of amorphous Boron Carbide (a-BxC) materials using Molecular Dynamics (MD) and Hybrid Reverse Monte Carlo (HRMC)", *J. Non-Crystalline Solids*, 530, 119783, (2020).
18. T. Qi, Y. Gong, A. Li, X. Ma, P. Wang, R. Huang, C. Liu, R. Sakidja, J. Z. Wu, R. Chen, L. Zhang, "Interlayer Transition in a vdW Heterostructure toward Ultrahigh Detectivity Shortwave Infrared Photodetectors", *Advanced Functional Materials*, v. 30[3], 1905687 (2020).
19. P. Adhikari, S. San, C. Zhou, R. Sakidja, W-Y Ching, "Electronic structure and mechanical properties of crystalline precipitate phases $M_{23}C_6$ ($M = Cr, W, Mo, Fe$) in Ni-based superalloys", *Materials Research Express*, 6[11], 116323, (2019).
20. J. Acharya, R. Goul, D. Romine, R. Sakidja, J. Z. Wu, "Effect of Al_2O_3 Seed-Layer on the Dielectric and Electrical Properties of Ultrathin MgO Films Fabricated using In Situ Atomic Layer Deposition", *ACS Applied Materials & Interfaces*, v. 11 [33], pp. 30368-30375, 2019 (2019).
21. T. Chen, R. Sakidja, W-Y Ching, C. Zhou, "Crystal Plasticity Modeling of Void Growth on Grain Boundaries in Ni-Based Superalloys", *JOM*, Nov. 2019, Vol. 71, Issue 11, pp 3859–386 (2019).
22. M. Alamri, R. Sakidja, R. Goul, S. Ghopry, and J. Z. Wu, "Plasmonic Au Nanoparticles on 2D MoS_2 /graphene van der Waals Heterostructures for High-Sensitivity Surface Enhanced Raman Spectroscopy", *ACS Applied Nano Materials*, 2 (3), pp. 1412-1420 (2019).
23. M. Gong, R. Sakidja, R. Goul, D. Ewing, M. Casper, A. Stramel, A. Elliot, and J. Z. Wu, "High-Performance All-Inorganic $CsPbCl_3$ Perovskite Nanocrystal Photodetectors with Superior Stability", *ACS Nano*, 13[2], pp. 1772-1783 (2019).
24. S. Ghopry, M. Alamri, R. Goul, R. Sakidja and J. Z. Wu, "Extraordinary Sensitivity of Surface-Enhanced Raman Spectroscopy of Molecules on MoS_2 (WS_2) Nanodomes/Graphene van der Waals Heterostructure Substrates", *Advanced Optical Materials*, 1801249, (2019).
25. Z. Zhang, R. Sakidja, F. Hu, B. Xu, S. Ren, "Self-Assembled Metal Molecular Networks by Nanoconfinement", *The Journal of Physical Chemistry Letters*, 10 [2], 206-213 (2019).
26. J. Wilt, R. Goul, J. Acharya, R. Sakidja, J. Z. Wu, "In situ atomic layer deposition and electron tunneling characterization of monolayer Al_2O_3 on Fe for magnetic tunnel junctions", *AIP Advances*, 8 [12], 125218, (2018).
27. Md Delower Hossain, R. Mayanovic, S. Dey, R. Sakidja, M. Benamara, "Room-Temperature Ferromagnetism in Ni(II)-Chromia based Core-Shell Nanoparticles: Experiment and First Principles Calculations", *Physical Chemistry Chemical Physics*, 20[15], pp. 10396-10406, (2018).
28. M. Gong, R. Sakidja, Q. Liu, R. Goul, D. Ewing, M. Casper, A. Stramel, A. Elliot and J. Z. Wu, "Broadband Photodetectors Enabled by Localized Surface Plasmonic Resonance in Doped Iron Pyrite Nanocrystals", *Adv. Optical Materials*, Vol. 6[8] 701241(2018). Featured as the back cover.
29. W. Ng, E. Gnanakumar, G. Rothenberg, E. Batyrev, S. Sharma, P. Pujari, H. Greer, W. Zhou, R. Sakidja, M. Barsoum and N. R. Shiju, "Ti₃AlC₂ MAX-phase as an efficient catalyst for oxidative dehydrogenation of n-butane", *Angewandte Chemie*, Vol. 130 [6], pp. 1501–1506 (2018).
30. Md. Delower Hossain, R. Mayanovic, R. Sakidja, M. Benamara and R. Wirth, "Magnetic properties of core-shell nanoparticles possessing a novel Fe(II)-chromia phase: an experimental and theoretical approach", *Nanoscale*, vol. 10, pp. 2138-2147 (2018).
31. J. Samantha Wilt, R. Sakidja, R. Goul and J. Z. Wu, "The effect of an interfacial layer on electron tunneling through atomically-thin Al_2O_3 tunnel barriers", *ACS Applied Materials and Interfaces*, 9[42], pp 37468– 37475 (2017).
32. D. G. Kizzire, S. Dey, R. A. Mayanovic, R. Sakidja, K. Landskron, M. Mandal, Z. Wang, M. Benamara, "Studies of the Mechanical and Extreme Hydrothermal Properties of Periodic Mesoporous Silica and Aluminosilica Materials", *Microporous and Mesoporous Materials*, [252], pp. 69–78 (2017).
33. J. Wilt, Y. Gong, M. Gong, F. Su, Huikai Xu, R. Sakidja, A. Elliot, R. Lu, S. Zhao, S. Han, and J. Z. Wu, "Atomically thin Al_2O_3 films for tunnel junctions", *Phys. Rev. Applied*, 7, 064022 (2017).
34. A. Ascone and R. Sakidja, "MDM2 Case Study: Computational Protocol Utilizing Protein Flexibility Improves Ligand Binding Mode Predictions", *Int. J. of Comp. Biology and Drug Design*, 10[3] pp. 207-224 (2017).

35. Md Shafiqul Islam, P. Simanjuntak, S. Mitra and R. Sakidja, "DFT Study on the Li Mobility in Li- Ion-Based Solid-State Electrolytes", *MRS Advances*, 1-6., 2 [54] (Energy Storage and Conversion), pp. 3277-3282 (2017).
36. M.D. Hossain, R. A. Mayanovic, R. Sakidja, M. Benamara "An experimental and theoretical study of the optical, electronic and magnetic properties of novel inverted α -Cr₂O₃ @ α -Mn_{0.35}Cr_{1.65}O_{2.94} core shell nanoparticles", *J. Materials Research*, 32[2], Jan. 2017, pp. 269-278, (2017).
37. B. Hunca, C. Dharmawardhana, R. Sakidja, and W-Y Ching, "Ab initio calculations of thermomechanical properties and electronic structure of Vitreloy Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni₁₀Be_{22.5}", *Phys. Rev. B*, 94, 144207 (2016).
38. D. G. Kizzire, J. Thomas, S. Dey, H. Osman, R. A. Mayanovic, R. Sakidja, Z. Wang, M. Mandal and K. Landskron, "Investigations of the Mechanical and Hydrothermal Stabilities of SBA-15 and Al-SBA-15 Mesoporous Materials", *MRS Advances*, 1[35] (Materials Design), pp. 2453- 2458, (2016).
39. S. Dey, S. Anderson, R. Mayanovic, R. Sakidja, K. Landskron, B. Kokoszka, M. Mandal, Z. Wang, "Experimental and theoretical investigation of a mesoporous KxWO₃ material having superior mechanical strength", *Nanoscale*, 8, pp. 2937-2943, (2016).
40. M. Gong, R. Sakidja, and S. Ren, "Composition and oxidation-controlled magnetism in ternary FeCoNi nanocrystals", *Nano Research*, 9 [3], pp. 831-836, (2016).
41. M. Gong, X. Jin, R. Sakidja, and S. Ren, "Synergistic strain engineering effect of hybrid plasmonic, catalytic and magnetic core-shell nanocrystals", *Nano Letters*, 12[15], pp. 8347-8353 (2015).
42. W. Qin, M. Gong, X. Chen, T. A. Shastry, R. Sakidja, G. Yuan, M. C. Hersam, M. Wuttig, and S. Ren, "Multiferroicity of Carbon-Based Charge Transfer Magnets", *Advanced Materials*, 27 [4], pp. 734-739 (2015). Featured as the front piece of the journal.
43. Q. Liu, Y. Gong, J. S. Wilt, R. Sakidja, J. Wu, "Synchronous growth of AB-stacked bilayer graphene on Cu by simply controlling hydrogen pressure in CVD process", *Carbon*, 93, pp. 199-206 (2015).
44. C. Dhakal, S. Aryal, R. Sakidja, W-Y Ching, "Approximate lattice thermal conductivity of MAX phases at high temperature", *J. European Ceramic Society*, 35[12], pp. 3203-3212 (2015).
45. S. Aryal, R. Sakidja, L. Ouyang, W-Y Ching, "Elastic and electronic properties of Ti₂Al (C_x N_{1-x}) solid solutions", *J. European Ceramic Society*, 35[12], pp. 3219-3227 (2015).
46. C. C. Dharmawardhana, R. Sakidja, S. Aryal, W-Y Ching, "In search of zero thermal expansion anisotropy in Mo₅Si₃ by strategic alloying", *J. Alloys and Compounds*, 620 [25], pp. 427-433 (2015).
47. N. Li, R. Sakidja and W-Y Ching, "Ab initio study on the adsorption mechanism of oxygen on Cr₂AlC (0001) surface", *Applied Surface Science*, 315 [1], pp. 45-54 (2014).
48. R. Sakidja, J. H. Perepezko and P. Calhoun, "Synthesis, Thermodynamic Stability and Diffusion Mechanism of Al₅Fe₂-Based Coatings", *Oxidation of Metals*, p. 1-11 (2014).
49. P. Downs, J. H. Perepezko, R. Sakidja and S. R. Choi, "Suppressing CMAS Attack with a MoSiB- Based Coating", *Surface and Coating Technology*, 239, pp. 138-146 (2014).
50. S. Aryal, R. Sakidja, M. W. Barsoum and W-Y Ching, "A genomic approach to the stability, elastic, and electronic properties of the MAX phases", *Physica Status Solidi (b)*, 251[8], pp. 1480-1497 (2014). Featured on the cover page.
51. N. Li, R. Sakidja, S. Aryal, W-Y Ching, "Densification of a continuous random network model of amorphous SiO₂ glass", *Physical Chemistry Chemical Physics*, 16[4], pp.1500-1514 (2014).
52. A. Bengtson, H. O Nam, S. Saha, R. Sakidja, D. Morgan, "First-principles molecular dynamics modeling of the LiCl-KCl molten salt system", *Computational Materials Science*, 83, 362-370 (2014).
53. H. O. Nam, A. Bengtson, K. Votler, S. Saha, R. Sakidja, D. Morgan, "First-principles molecular dynamics modeling of the molten fluoride salt with Cr solute", *J. Nuclear Materials*, 449 [1-3], 15, pp. 148-157 (2014).
54. C. C. Dharmawardhana, R. Sakidja, S. Aryal, W-Y Ching, "Temperature dependent mechanical properties of Mo-Si-B compounds via ab-initio molecular dynamics", *APL Materials*, 1, 012106 (2013).
55. N. Li, R. Sakidja, W-Y Ching, "Oxidation of Cr₂AlC (0001): Insights from Ab Initio Calculations", *Journal of Metals (JOM)*, 65[11], pp 1487-1491 (2013).
56. P. Ritt, O. Lu-Steffes, R. Sakidja, J. H. Perepezko, W. Lenling, D. Crawmer, J. Beske "Application of Plasma Spraying as a Precursor in the Synthesis of Oxidation-Resistant Coatings", *Journal of Thermal Spray Technology*, 22[6], pp. 992-1001 (2013).

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81. R. Sakidja, H. Sieber, and J. H. Perepezko, "The formation of Mo precipitates in a supersaturated Mo₅SiB₂ intermetallic phase", *Phil. Mag. Letter*, 79, pp. 351-362 (1999).

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83. R. R. Schartman, R. Sakidja and E. E. Hellstrom, "Supersolidus Phase Investigation of the Bi-Sr- Ca-Cu Oxide System in Silver Tape", *Journal of American Ceramic Society*, 76 [3], pp.724-728 (1993).

Conference Proceedings:

1. Razib Iqbal, Taylor Kuttentkuler, Chad Brewer, R. Sakidja," A Framework for Visualizing the Dynamic Events of Carbon Nanocomposites using Virtual and Augmented Reality Tools", Proceedings of the 16th International Joint Conference on e-Business and Telecommunications (ICETE 2019), pp. 331-336 ISBN: 978-989-758-378-0.
2. S. Im, M. M. Paquette, M. Belhadj-Larbi, P. Rulis, R. Sakidja & J. Hwang, "Nanoscale Structure-Property Relationship in Amorphous Hydrogenated Boron Carbide for Low-k Dielectric Applications", *Microscopy and Microanalysis*, 23(S1), 1486-1487 (2017).
3. J. H. Perepezko, S. D. Imhoff, R. Sakidja, "Analysis and Control of Interface Reactions in Microelectronic Systems", *International Symposium on Microelectronics*, (1), 000264-000274 (2011).
4. A. P. Alur, R. Sakidja, P Wang, P Jain, J. H. Perepezko, KS Kumar, "Deformation Behavior of a Quaternary Mo-Nb-Si-B Alloy", *MRS Proceedings 1295*, mrsf10-1295-n07-03 (2011).
5. J. H. Perepezko, R. Sakidja, "Oxidation Response and Coatings for Mo-Si-B Alloys", *MRS Proceedings 1295*, mrsf10-1295-n07-01 (2011).
6. J. H. Perepezko, K. Hildal, F. Rioult, R. Sakidja, Enhanced oxidation resistance of high temperature Mo-Si-B alloys, 17th International Corrosion Congress (2008).
7. R. Sakidja, J. Werner, J. H. Perepezko, "Borosilicide Coatings for High-Temperature Mo-Si-B Alloys", *Surface Modification Technologies: Proceedings of the 19th International Conference on Surface Modification Technologies*, August 1-3, 2005, Radisson Riverfront Hotel, St. Paul, Minnesota, USA, p. 134, ASM International (2006).
8. N. Sekido, R. Sakidja, J. H. Perepezko, "Nucleation of (Mo) Precipitates on Dislocations during Annealing of a Mo-rich Mo₅SiB₂ Phase", *MRS Proceedings 842*, S5. 35 (2004).
9. R. Sakidja, J. H. Perepezko, "Microstructure Development in High-Temperature Mo-Si-B Alloys", *MRS Proceedings 851*, NN11. 11 (2004)
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11. R. Sakidja, S Kim, J. S. Park, J. H. Perepezko, "Transition Metal Alloying and Phase Stability in the Mo-Si-B System", *MRS Proceedings 753*, BB2. 3 (2002).
12. J. H. Perepezko, R. Sakidja, S. Kim, Z. Dong, J. S. Park," Multiphase microstructures and stability in high temperature Mo-Si-B alloys", *Third International Symposium on Structural Intermetallics*, 505-514(2001).
13. S. Kim, R. Sakidja, Z. F. Dong, J. H. Perepezko, Y. W. Kim, "Growth of the Mo₅SiB₂ Phase in a Mo₅Si₃/Mo₂B Diffusion Couple", *MRS Proceedings 646*, N5. 42.1 (2000).
14. J. H. Perepezko, R. Sakidja, S. Kim, "Phase stability in processing and microstructure control in high temperature Mo-Si-B alloys", *MRS Proceedings 646*, N4. 5.1 (2000).
15. R. Sakidja, H. Sieber, J. H. Perepezko, *Molybdenum & molybdenum alloys*, TMS, Warrendale, p. 99 (1998).
16. R. Sakidja, G. Wilde, H. Sieber, J. H. Perepezko, "Microstructural development of Mo (ss)+ T₂ two-phase alloys", *MRS Proceedings 552*, KK6. 3.1 (1998).
17. C. A. Nunes, R. Sakidja, J. H. Perepezko, "Phase stability in high-temperature Mo-rich Mo-B-Si alloys", *Structural Intermetallics*, 831-839 (1997).

Book Chapters:

- R. Sakidja and J. H. Perepezko, "Phase Stability in Refractory Metal Silicides", in *The Science of Complex Alloy Phases*, edited by Thaddeus B. Massalski and Patrice E. Turchi, ISBN: 978-0- 87339-593-9 (John Wiley & Sons, 2010), pp. 373-408.

- J. H. Perepezko, R. Sakidja and K. S. Kumar, "Mo-Si-B Alloys for Ultrahigh Temperature Applications", Chapter 13 in *Advanced Structural Materials: Properties, Design Optimization, and Applications*, edited by W. Soboyejo (CRC Press, Boca Raton, FL, 2007) pp. 437 - 473.

Advising Activities:

Current graduate student advisees:

- Tony Astuhuaman Davila, MS student in MNAS Interdisciplinary Program, Topic: Development of an End-to-End Generative AI Workflow for Drug Discovery: From Structure-Based Design to Blind Docking and Molecular Dynamics.
- Gaige Riggs, MS student in 1) Materials Science Program, Topic: Applications of Generative Artificial Intelligence to molecular docking and drug design and 2) Natural and Applied Science Interdisciplinary Program, Topic: Development of Quantum Circuit Simulations to Model Surface Chemistry Dynamics.
- Matthew D. Bruenning, MS student in Materials Science Program, Topic: AI applications to model the corrosion behavior in Molten Salt Reactor (MSR).
- Anika Tabassum, MS Student in Materials Science Program, Topic: Development of MLIP to model Atomic Layer Deposition for Superconducting Qubits.

Current undergraduate student advisees:

- Seungmin (Rachel) Lee, BSc in Physics. Topic: AI applications to model ALD for Superconducting Qubits.
- Jonathan Kliewer, BSc in Physics. Topic: AI applications to model Shape Memory Alloys (Nitinol).
- Helena Bel, BSc in Physics. Topic: AI applications to model structural materials in golf shafts.

Advised graduate students and served as a committee chair of their MS theses:

- Marium Mostafiz Mou, MS student in Materials Science Program, Topic: Interatomic Potential Development for Ni-based Superalloys. Mou defended her thesis in Spring of 2023 and is currently a PhD student in Materials Science at *North Carolina State University-Raleigh*.
- Nur Aziz Octoviawan, MS student in Materials Science Program, Topic: Interatomic Potential Development for High-Entropy driven Diborides. Aziz defended his thesis in Spring 2023 and is currently a PhD student in Materials Science at *Washington University at St. Louis*.
- Devon Romine, MS student in Materials Science, Topic: Reactive Molecular Dynamics Simulations on Atomic Layer Depositions (ALD) of Ultrathin Tunnel Barriers. Mr. Romine defended his thesis and graduated with an MS degree in Materials Science in Spring 2022. He is a Lecturer at *Missouri State University*.
- Emily Justus, MS student in Materials Science, Topic: Artificial Intelligence (AI) Applications on the Kinetic Monte Carlo (kMC) Simulations of Atomic Layer Depositions (ALD). Ms. Justus defended her thesis and graduated with an MS degree in Materials Science in Spring 2022. She works as a Quality Engineer at *Eagle-Picher Technologies*.
- Alin Niraula, MS student in Materials Science, "Thermal Property Modeling of High-Temperature Diborides". Mr. Niraula defended his thesis and graduated with an MS degree in Materials Science in Spring 2021. He is currently a PhD student in Physics at *Louisiana State University*.
- Bikash Timalina, MS student in Materials Science, "Interatomic Potential Development for High-Temperature Diborides". Mr. Timalina defended his thesis and graduated with an MS degree in Materials Science in Spring 2021. He is currently a PhD student in Mechanical Engineering at the *University of Virginia*.
- Kwabena Asante-Boahen, "Reactive Molecular Dynamics Modeling in Low-temperature Synthesis of Amorphous Boron Carbide". Mr. Asante-Boahen defended his thesis and graduated with an MS degree in Materials Science in Spring 2021. He is currently a PhD student in Nanoengineering at *North Carolina A&T*.
- David T Magness, "Kinetic Monte Carlo Modeling in Atomic Layer Deposition (ALD) of Ultrathin Tunnel Barriers". Mr. Magness defended his thesis on Nov. 17th, 2020, and graduated with an MS degree in Materials Science in Fall 2020.
- Yuxuan Lu "Reactive MD simulation on the formation of amorphous sub-nano alumina layer using atomic layer deposition (ALD)". Ms. Lu defended her thesis on July 15th, 2020 and graduated with an MS degree in Materials Science in SU20.

- Sabila Kader Pinky “Molecular Dynamics (MD) Study of Creep Deformation in Nickel-Based Superalloys”. Ms. Pinky defended her thesis on Nov. 13th, 2019, and graduated with an MS Degree in Materials Science in FA19. She is currently pursuing a PhD in Materials Science at the *North Carolina State University-Raleigh*.
- Muztoba Rabbani “Development of Multi-component EAM Potential for Ni-based Superalloys”. Mr. Rabbani defended his thesis on Nov. 13th, 2019 & graduated with an MS Degree in Materials Science in FA19. He is currently pursuing a PhD in Materials Science at the *University of California- Merced*.
- Rajan Khadka, “Study of amorphous boron carbide (a-B_xC) and hydrogenated boron carbide (a-B_xC:H_y) using Molecular Dynamics and Hybrid Reverse Monte Carlo”. Mr. Khadka defended his thesis on Nov. 14th, 2019 & graduated with an MS Degree in Materials Science in FA19. He is currently pursuing a PhD in Materials Science at the *Rensselaer Polytechnic University*.
- Nirmal Baishnab "Synthesis of Amorphous Hydrogenated Boron Carbide from Orthocarborane using Argon Bombardment: A ReaxFF Molecular Dynamics Study". Mr. Baishnab defended his thesis on July 18th, 2019, and graduated with an MS degree in Materials Science in SP19. He is currently pursuing a PhD in Electrical Engineering at *Iowa State University*.
- Md. Shafiqul Islam “DFT Study on the Li Mobility in Li-Ion-Based Solid-State Electrolyte”, Mr. Islam successfully defended his thesis on Nov. 30th, 2017, and graduated with an MS degree in Materials Science in FA17. He obtained a PhD in Materials Science at the *University of Maryland at College Park*.
- Paul Simanjuntak “Development of Many-Body Potential for Deformation Study in Al-TiN Nanolayered Composites”. Mr. Simanjuntak defended his thesis on April 18th, 2017, and graduated with an MS degree in Materials Science in SP17. He obtained a PhD in Mathematics at the *University of Missouri at Columbia* and is currently a Visiting Assistant Professor at *UT-Austin*.
- Anthony Ascone “MDM2 Case Study: Computational Protocol Utilizing Protein Flexibility Improves Ligand Binding Mode Predictions”. Mr. Ascone defended his thesis on July 28th, 2016, and graduated with an MS degree in Materials Science (FA16).

Co-advised graduate students on the atomistic modeling aspects of their MS theses:

- Mohammad Delower Hossain, “Experimental and Theoretical Analysis of the Structural, Electronic and Magnetic Properties of Novel Inverted Core-Shell-Cr₂O₃@-MXCr₂-XO₃-Y (M=Co, Ni, Mn, Fe) Nanoparticles”. MS Thesis Adviser: Robert Mayanovic.
- Dayton Gage Kizzire, “An Experimental and Computational Investigation of the Mechanical, Structural and Hydrothermal Properties of Mesoporous Materials”. MS Thesis Adviser: Robert Mayanovic.
- Priyanka Karnati, “A Study on Structural and Optical Properties of Vertically Aligned Zinc Oxide Nanorods”. MS Thesis Adviser: Kartik Ghosh.

Advised undergraduate students in Physics on their senior research projects:

- Maverick Stover: Developing Neural Network Interatomic Potentials for Molten Salts.
- Matthew Kindhart: Machine Learning Efficiency: A Study in Conserving Computer Resources.
- William Brockmeier: A study and model of meteor-like collisions.
- Austin Bollinger: A Study of Molecular Dynamics Simulations of Metallic Systems.
- Greg Luckey: Using LAMMPS to simulate large-scale impacts.
- Christopher Robledo: Virtual reality applications for simulations of carbon-based nanocomposites.
- Eiad Hamwi: Modeling the migration and accumulation of smooth muscle cells on blood vessels.
- Woosung Lee: Molecular dynamics investigation of mesoporous silica.
- Timothy Stillings: Atomistic modeling of bonding in carbon-based nanostructures.

Advised undergraduate students in Physics on their presentations:

- Jonathan Kliewer and Ridwan Sakidja, “Nitinol Interatomic Potential Using Moment Tensor Potentials in Machine Learning”, American Physics Society (APS) March Meeting, Minneapolis, MN, March 4-8, 2024.
- Seungmin (Rachel) Lee and Ridwan Sakidja, “Development of Artificial Intelligence-Based Forcefields to Model Tunnel Barriers In Superconducting Qubits”, American Physics Society (APS) March Meeting, Minneapolis, MN, March, 4-8, 2024.

- Seungmin (Rachel) Lee, Gaige Riggs, Ridwan Sakidja, “Development of Artificial Intelligence-Based Potentials”, Poster presentation at 2023 American Physical Society (APS) Fall Meeting – Prairie Section. (Dec 1st, 2023). ** Selected for Student Presentation Prize Awards.
- Rachel Lee and Ridwan Sakidja, “Development of Artificial Intelligence-based Forcefields to Model Tunnel Barriers in Superconducting Qubits”, Poster presentation at 2023 CNAS Undergraduate Research Day (April 28th, 2023). ** won second place for Physics, Astronomy & Materials Science category.
- Tyler McGilvry-James and Ridwan Sakidja, “Artificial Intelligence for Defect Examination”, Poster presentation at 2021 CNAS Undergraduate Research Day. ** won second place for Physics, Astronomy & Materials Science category.
- Tyler McGilvry-James, Andrew Duff, Bikash Timalsina, Alin Niraula, Muztoba Rabbani, Nirmal Baishnab, Puja Adhikari, Saro San, Wai-Yim Ching, Ridwan Sakidja, "Development of Reference-free (RF) MEAM Interatomic Potentials for Transition Metal-rich Carbides", American Physics Society (APS) March Meeting, March 15-19, 2021, Virtual Meeting.
- Tyler McGilvry-Jame, “Reference-free Interatomic Potential Development and Modeling of Transition Metal Carbides”, Poster presentation at 2020 CNAS Undergraduate Research Symposium.
- Austin Bollinger, “Molecular Dynamics Simulations of Metallic Systems”, Poster presentation at CNAS Undergraduate Research Day (May 3rd, 2019). ** won first place for Physics, Astronomy & Materials Science category.
- Tyler McGilvry-James, “Molecular Dynamics (MD) Potential Development for Carbides”, Poster presentation at CNAS Undergraduate Research Day (May 3rd, 2019).
- Devon Romine, Chris Klenke, Daniel Fishbein, “Molecular Dynamics Simulations to Study Tunnel Barrier Layer Formation in Ultra-thin Film Alumina”, Poster presentation at CNAS Undergraduate Research Day (May 3rd, 2019).
- Greg Luckey and Devon Romine, “Adapting Molecular Dynamics Hydrocode to Simulate Large Scale Oblique Impact Structures”, Oral presentation at the 28th Annual Spring Meeting of the NASA-Missouri Space Grant Consortium, held at the Missouri University of S&T, Rolla MO, April 26-27, 2019. Co-advisors: R. Sakidja and K. Evans.
- Daniel Fishbein, Devon Romine, and Greg Luckey, “Application of Hydrocode Modeling to Model Low-Angle Terrestrial Impacts”, Poster presentation at the 28th Annual Spring Meeting of the NASA-Missouri Space Grant Consortium, held at the Missouri University of S&T, Rolla MO, April 26-27, 2019.
- Daniel Fishbein and Devon Romine, "Modeling Atomic Layer Deposition of Alumina as an Ultra- thin Tunnel Barrier", Poster presentation at the Arkansas IDeA Network of Biomedical Research Excellence (INBRE), Nov. 2-3, 2018, Fayetteville, AR.
- (Invited Student Presentation) Christopher Klenke, Devon Romine & Daniel Fishbein, “Molecular Dynamic Simulations to Study Tunnel Barrier Layer Formation in Ultra-Thin Film Alumina", Oral presentation at the Arkansas IDeA Network of Biomedical Research Excellence (INBRE), Nov. 2- 3, 2018, Fayetteville, AR. ** won the second place for Physics Undergraduate Category.
- Austin Bollinger, "Molecular Dynamic Simulations of Layered Metallic Systems", Poster presentation at the Arkansas IDeA Network of Biomedical Research Excellence (INBRE), Nov. 2-3, 2018, Fayetteville, AR.
- Tyler McGilvry-James, "Molecular Dynamics (MD) Potential Development for Carbides". Poster presentation at the Arkansas IDeA Network of Biomedical Research Excellence (INBRE), Nov. 2- 3, 2018, Fayetteville, AR.
- Chad Brewer, Taylor Kuttenkuler, Brittany Porter & Chris Klenke, "Visualizing the Critical Dynamic Events of Carbon Nanocomposites Using Low-Cost Wearable Virtual Reality Tools". Poster presentation at the 27th Annual Spring Meeting of the NASA-Missouri Space Grant Consortium, held at the Missouri University of S&T, Rolla MO, April 20-21, 2018. Co-advisors:R. Iqbal and R. Sakidja.
- Eiad Hamwi, "Modeling the Effect of Hemodynamic Forces on the Migration of Smooth Muscle Cells Towards Blood Vessels". Poster presentation by at Arkansas INBRE, Oct. 27-28, 2017, Fayetteville, AR. Co-advisors: Ryan Udan and R. Sakidja.

- Christopher Robledo, "Virtual Reality Applications for Simulations in Carbon-Based Nanocomposites". Poster presentation by at Arkansas INBRE, Oct. 27-28, 2017, Fayetteville, AR.
- Jesse Underwood, "Computational Investigations of Hydrous Aluminosilicate Melts". Poster presentation by at Arkansas INBRE, October 27-28, 2017, Fayetteville, AR. Co-advisors: R. Mayanovic and R. Sakidja.
- (Invited Student Presentation) Austin Bollinger, "Molecular Dynamics Simulations of Layered Metallic Systems". Oral presentation by at Arkansas INBRE, Oct. 27-28, 2017, Fayetteville, AR
- Jesse Underwood, "Experimental and Computational Investigations of Hydrous Aluminosilicate Melts", Poster presentation at 2017 CNAS Undergraduate Research Day (May 2nd 2017). Co- advisors: R. Mayanovic and R. Sakidja. ** won second place for Physics, Astronomy & Materials Science category.
- Eiad Hamwi, "Modeling the Role of Hemodynamic Forces in the Formation of Smooth Muscle Cell (VCMCS) around Proximal Arteries", Poster presentation at 2017 CNAS Undergraduate Research Day (May 2nd, 2017). Co-advisors: R. Udan and R. Sakidja.
- Jesse Underwood, "Experimental and Computational Investigations of Hydrous Aluminosilicate Melts", Oral Presentation at the 26th Annual Meeting of the NASA-Missouri Space Grant Consortium (April 21-22, 2017). Co-advisors: R. Mayanovic and R. Sakidja.
- Nicholas Delomora and Brittany Porter, "Augmented Reality Application for Carbon Nanostructures", Poster presentation at the 26th Annual Meeting of the NASA-Missouri Space Grant Consortium (April 21-22, 2017).
- Chris Robledo and Matt Yaeger, "Virtual Reality Application for Carbon Nanostructures", Oral Presentation at the 26th Annual Meeting of the NASA-Missouri Space Grant Consortium (April 21-22, 2017).
- (Invited Student Presentation) Jesse Underwood, Dayton G. Kizzire, J. Thomas, "Molecular Dynamics Simulations of the Mechanical and Structural Properties of Silica and Aluminosilica Mesoporous Materials" Oral presentation at Arkansas INBRE 2016, Oct. 21-22, 2016, Fayetteville, AR. Co-advisors: R. Mayanovic & R. Sakidja. Won 1st place for Physics Undergraduate Category.
- Jamie Thomas, "Computational Modeling of the Mechanical and Hydrothermal Stabilities of Mesoporous Materials" Poster presentation at 2016 CNAS Undergraduate Research Day (April 21st, 2016). Co-advisors: R. Mayanovic & R. Sakidja.
- Tim Stillings, "Atomistic Modeling of Bonding in Carbon-based Nanostructures", Poster presentation at 2016 CNAS Undergraduate Research Day (April 21st, 2016).
- Kent Mastroianni, "The Effects of Nanoparticle Size on the Properties of Simulated SiO₂ Melts" Poster presentation at 2016 CNAS Undergraduate Research Day (April 21st, 2016).
- Zach Leuty, "Aluminide Diffusion Coatings ", Poster presentation at 2016 CNAS Undergraduate Research Day (April 21st, 2016).
- Gavin Hester, "Molecular Dynamics Study of Lithium-Ion Conducting Phosphate Glass", Poster presentation at 2016 CNAS Undergraduate Research Day (April 21st, 2016). Co-advisors: S. Mitra and R. Sakidja. ** won first place for Physics, Astronomy & Materials Science Category.
- Timothy Stillings, "Report on Atomistic Modeling of Bonding in Carbon-Based Nanostructures", Oral presentation at the 25th Annual Meeting of the NASA-Missouri Space Grant Consortium (April 22-23, 2016), Rolla, MO.
- Zach Leuty, "Comparison of Aluminide Diffusion Coatings on Various Steel Substrates Synthesized by Pack Cementation", Oral presentation at the 25th Annual Meeting of the NASA- Missouri Space Grant Consortium (April 22-23, 2016), Rolla, MO.
- (Invited Student Presentation) Zach Leuty, "Aluminide Diffusion Coatings" at Arkansas INBRE 2015, Friday, November 6th, 2015, Fayetteville, AR.

Presentations:

Underlined: graduate students as a first author/ presenter

- (Invited) "Advancements in Interatomic Potential Development for High Entropy Materials", October 7th, 2024, MS&T 2024, Pittsburgh, PA.
- Matthew D Bruening and Ridwan Sakidja, "Development of MLIP to model corrosion behavior in Molten Salt Reactors" at the *APS March Meeting 2024*, Minneapolis, MN.

- Gaige Riggs and Ridwan Sakidja, “Convolutional Neural Network Analysis of Molecular Docking for Cancer Drug Discovery” at the *APS March Meeting 2024*, Minneapolis, MN.
- Matthew D Bruening, Gaige Riggs, Jonathan Kliewer and Seungmin (Rachel) Lee, “Development of Mediator Assisted N' GNN Optimization (MANGO) Project” to be presented at the *APS March Meeting 2024*, Minneapolis, MN.
- (Invited) “Development of Machine Learning Interatomic Potentials to Model Materials Processing & Performance in Multicomponent Systems”, Oct. 4th, 2023, at *MS&T 2023*, Columbus, OH.
- Ridwan Sakidja, "Use of applied mathematics in artificial neural networks (ANN) to model advanced and complex materials", Saturday, April 1st, 2023, at *2023 Mathematical Association of America, Missouri Section Meeting* held in Missouri State University.
- Ridwan Sakidja, Hendra Hermawan, Ayoub Tanji, Peter K Liaw and Xuesong Fan, "Development of Deep Learning Potentials to Investigate Initial Corrosion Mechanisms", Session EE02: V: Machine Learning in Physics 10:00 AM–12:00 PM, March 20th, *APS March Meeting 2023*.
- Nur Aziz Octoviawan, Gregory E Hilmas, William G Fahrenholtz and Ridwan Sakidja, "Development of Artificial intelligence-based Interatomic Potentials High-Entropy Diborides for Modelling the Physical and Thermal Properties", Session N20: Matter at Extreme Conditions: Simulation and Novel Methods, 11:30 AM–2:18 PM, Wed., March 8th, *APS March Meeting 2023*.
- Marium M. Mou, Matthew J. Kindhart, Jared L Shortt and Ridwan Sakidja, "Development strategies and hyperparameter optimization of Deep Learning potentials for multi-component and multi-phase Nickel-based Superalloys", Session N53: AI and Materials III 11:30 AM–2:30 PM, March 8th, *APS March Meeting 2023*.
- (Invited) Ridwan Sakidja, "Development of Machine Learning Potentials for Multicomponent Systems", *Chemistry Dept. Seminar, Missouri University of Science and Technology*, Rolla, MO, March 13th, 2023.
- (Invited) R. Sakidja and M. Mou, "Alloying Design and Deep Learning Applications for Concentrated and High-entropy-Driven Ni-based Superalloys", Symposium on the Integration between Modeling and Experiments for Crystalline Metals: From Atomistic to Macroscopic Scales IV, *MS&T 2022*, Pittsburgh, PA, October 9-12, 2022.
- Devon T Romine, R. Sakidja, J. Z. Wu, "Modeling Atomic Layer Deposition of Alumina as an Ultra-thin Tunnel Barrier using Reactive Molecular Dynamics", Session D66: Adsorption, Growth and Catalysis, March 14th, *APS March Meeting 2022*.
- Nur Aziz Octoviawan, B. Timalsina, G. E Hilmas, W. G Fahrenholtz, R. Sakidja, "Deep-Learning Potentials to Simulate Thermo-Mechanical and Physical Behavior of Entropy-Driven Diborides", American Physics Society, Session F24: Matter at Extreme Conditions: Simulations, March 15th, *APS March Meeting 2022*.
- Tyler McGilvry-James, M. M. Mou, R Sakidja, "Deep Potential Development of Highly Concentrated/High Entropy-driven Carbides", American Physics Society (APS) March Meeting, Session N49: Emerging Trends in Molecular Dynamics Simulations and Machine Learning III, March 16, *APS March Meeting 2022*.
- Marium Mostafiz Mou, T. J McGilvry-James, R. Sakidja, "Machine learning strategies for potential development in highly concentrated/high-entropy driven Ni-based Superalloys", Session Q46: Emerging Trends in Molecular Dynamics Simulations and Machine Learning II, March 16, 2022, APS March Meeting 2022.
- Nur Aziz Octoviawan, B. Timalsina, W. Fahrenholtz, G. Hilmas, R. Sakidja, "Development of Deep Learning Potentials for Zirconium and High-Entropy Stabilized Diborides", *46th International Conference and Expo on Advanced Ceramics and Composites (ICACC-2022)*.
- R. Sakidja, A. Niraula, B. Timalsina, W. Fahrenholtz, G. Hilmas, "Modeling the transport properties of high entropy-stabilized diborides", *46th International Conference and Expo on Advanced Ceramics and Composites (ICACC-2022)*.
- Tyler McGilvry-James, B. Timalsina, A. Duff, N. Baishnab, P. Adhikari, S. San, W-Y Ching, R. Sakidja, "Development of Deep and RF-MEAM Potentials to Model Physical and Thermo- Mechanical Properties of Metal-Rich Carbides", Symposium DS03—Combining Machine Learning with Simulations for Materials Modeling, *MRS Fall 2021 Meeting*, Boston, No. 29-Dec.2, 2021.

- Emily Justus, D. Magness, B. Timalisina, J. Z. Wu, Ridwan Sakidja, "Applications of a Combined Approach of Kinetic Monte Carlo Simulations and Machine Learning to Model Atomic Layer Deposition (ALD) of Metal Oxides", Symposium SF01—Advanced Atomic Layer Deposition and Chemical Vapor Deposition Techniques and Applications, *MRS Fall 2021 Meeting*, Boston, No. 29-Dec.2, 2021.
- Devon Romine, Y. Lu, J. Z. Wu, R. Sakidja. "Modeling Atomic Layer Deposition of Alumina as an Ultra-Thin Tunnel Barrier Using Reactive Molecular Dynamics", Symposium SF01— Advanced Atomic Layer Deposition and Chemical Vapor Deposition Techniques and Applications, *MRS Fall 2021 Meeting*, Boston, No. 29-Dec.2, 2021.
- (Invited) Ridwan Sakidja, Andrew Duff; Bikash Timalisina, Tyler McGilvry-James, "Development of Interatomic Potentials for Highly Concentrated/Entropy-stabilized Systems", Symposium on High Entropy Materials: Concentrated Solid Solutions, Intermetallics, Ceramics, Functional Materials and Beyond II. *MS&T 2021*, Columbus, OH, October 17 -21, 2021.
- (Invited) Ridwan Sakidja, Andrew Duff, Wai-Yim Ching, Caizhi Zhou, "Development of Interatomic Potentials to Model the Deformation Behaviors in Highly Concentrated/Entropy- stabilized Ni-base Superalloys", High Entropy Alloys IX: Structures and Modeling Symposium, *2021 TMS Annual Meeting and Exhibition*, March 15 -18, 2021, Virtual Meeting.
- Bikash Timalisina, Alin Niraula, Andrew Duff, Gregory Hilmas, William Fahrenholtz, Ridwan Sakidja, "Development of RF-MEAM interatomic potentials for high temperature diborides", March 15-19, 2021, *Virtual APS March Meeting 2021*.
- Devon Romine, Ridwan Sakidja, Judy Wu, Yuxuan Lu, "Modeling Atomic Layer Deposition of Alumina as an Ultra-thin Tunnel Barrier using Reactive Molecular Dynamics", March 15-19, 2021, *Virtual APS March Meeting 2021*.
- A Niraula, B Timalisina, G Hilmas, W Fahrenholtz, R Sakidja, "Theoretical calculations on transport properties of high-temperature binary and entropy-stabilized diborides", March 15-19, 2021, *Virtual APS March Meeting 2021*.
- D. Magness, E Justus, B Timalisina, J Wu, R Sakidja, "Applications of Kinetic Monte Carlo Simulations and Machine Learning to model Atomic Layer Deposition (ALD) of Metal Oxides", March 15-19, 2021, *Virtual APS March Meeting 2021*.
- K Asante Boehen, N. Baishnab and R. Sakidja, "Modeling the Argon bombardment and densification of Low-Temperature Organic Precursors using Reactive Molecular Dynamics Simulations and Machine Learning", March 15- 19, 2021, *Virtual APS March Meeting 2021*.
- Alin Niraula, B. Timalisina, G. Hilmas, W. Fahrenholtz, R.Sakidja, "Transport properties of binary and entropy-stabilized diborides", *45th International Conference and Exposition on Advanced Ceramics and Composites (ICACC)*, Feb. 8-12, 2021, Virtual Meeting.
- Bikash Timalisina, Alin Niraula, Andrew Duff, Gregory Hilmas, William Fahrenholtz, Ridwan Sakidja, "EAM and RF-MEAM potentials for thermal properties of zirconium diboride", *45th International Conference and Exposition on Advanced Ceramics and Composites (ICACC)*, Feb. 8-12, 2021, Virtual Meeting.
- R. Sakidja, Rajan Khadka, N. Baishnab and G. Opletal, "Development of Reactive Molecular Dynamics (MD) and Hybrid Reverse Monte Carlo (HRMC) Modeling to Synthesize Amorphous Boron Carbide", *TMS Annual Meeting & Exhibition 2020*, Feb 23-27, 2020, San Diego, CA.
- R. Sakidja, Devon Romine, Jagaran Archarya, Ryan Goul, Judy Wu, "Use of Atomistic-based Modeling and Materials Informatics to Design and Synthesize Ultra-thin Tunnel Junctions", *TMS Annual Meeting & Exhibition 2020*, Feb 23 - 27, 2020, San Diego, CA.
- (Invited) R. Sakidja and Wai-Yim Ching, "Compositional Design and Deformation Behavior in Ni-based Concentrated/HEA Alloys", *TMS Annual Meeting & Exhibition 2020*, Sun, Feb 23-27 2020, San Diego, CA.
- R. Sakidja, "Development of Interatomic Potentials and MD Simulations to Model the Deformation Behaviors in Ni-base Superalloys", *2019 eXtremeMAT National Laboratory Consortium (XMAT) Workshop*, hosted by Los Alamos National Laboratory, Dec. 4-5, 2019, Los Alamos, NM.
- R. Sakidja and W-Y Ching, "Compositional Design, Elongation and Dislocation Mobility in HEA Alloys" *World Congress on High Entropy Alloys (HEA 2019)*, November 17-20, 2019, Seattle, WA.

- Sabila Kader Pinky and Ridwan Sakidja, "Void Growth in Bicrystalline and Polycrystalline Ni- based Superalloy: Atomistic Calculation", *MS&T 2019*, Sept. 29–October 3, 2019, Portland, OR.
- Muztoba Rabbani, Sabila Kader Pinky, Nirmal Baishnab, Tyler McGilvry James, Ridwan Sakidja, "Development of EAM Interatomic Potentials of Aluminides and Carbides for Ni-based Superalloys, at the *MS&T 2019*, September 29–October 3, 2019, Portland, OR.
- R. Sakidja, W-Y Ching and C. Zhou, "Multimodal Approach to Modeling Creep Deformation in Ni-base Superalloys", at *2019 NETL Annual Review Meeting for Crosscutting Research*, April 9 -12, 2019, Pittsburgh, PA.
- (Invited) "The Use of Atomistic-Based Modeling and Informatics to Design and Synthesize Complex and Novel Materials", *Seminar Talk in the Dept. of Materials Science & Engineering in Michigan Technological University*, Feb. 18th, 2019, Houghton, MI.
- (Invited) "The use of ab-initio and classical molecular dynamics modeling to design and synthesize complex disordered solid structures", at the *43rd International Conference & Expo on Advanced Ceramics and Composites (ICACC 2019)*, 1/27 – 2/1, 2019, Daytona Beach, FL.
- Rajan Khadka, N. Baishnab, P. Rulis, J. Hwang, M. Paquette, N. Oyler, G. Opletal and R. Sakidja "The structure of amorphous hydrogenated boron carbide (a-BC:H) studied using a Hybrid Reverse Monte Carlo algorithm (HRMC)", at the *43rd International Conference & Expo on Advanced Ceramics and Composites (ICACC 2019)*, 1/27 – 2/1, 2019, Daytona Beach, FL.
- Nirmal Baishnab, R. Khadka, P. Rulis and R. Sakidja, "Molecular Dynamics Simulation Study on Synthesis and Characterization of Boron Carbide from Orthocarborane", at the *43rd Inter. Conference & Expo on Advanced Ceramics and Composites (ICACC 2019)*, 1/27 – 2/1'19, Daytona Beach, FL.
- R. Sakidja, B. Hunca, C. Dharmawardhana, and W-Y Ching, "On the Connection between the Electronic Structure and the Thermomechanical Properties of Zr-based Bulk Metallic Glass", *MS&T 2018*, Oct. 14-18, 2018, in Columbus, OH.
- N. Baishnab, R. Khadka and R. Sakidja, "Molecular Dynamics Simulation Study on Amorphous B₄C", *MS&T 2018*, Oct. 14-18, 2018, in Columbus, OH.
- R. Khadka, N. Baishnab and R. Sakidja, "Atomistic Modelling of Amorphous Boron Carbide Materials (B₄C)", *MS&T 2018*, Oct. 14-18, 2018, in Columbus, OH.
- M. Rabbani, N. Baishnab, S. K. Pinky and R. Sakidja, "Development of multi-component EAM potential for Ni-based Superalloys", *MS&T 2018*, Oct. 14-18, 2018, in Columbus, OH.
- S. K. Pinky, M. Rabbani and R. Sakidja, "Molecular Dynamics Study of Creep Deformation in Nickel-based Superalloys", *MS&T 2018*, Oct. 14-18, 2018, in Columbus, OH.
- (Invited) "The use of molecular dynamics and hybrid reverse Monte Carlo modeling to design and synthesize complex disordered solid structures", *Seminar at Dept. of Physics, University of Kansas*, Sept. 27th, 2018.
- Menglin Zhu, Soohyun Im, Michelle Paquette, Nathan Oyler, Paul Rulis, Ridwan Sakidja, Jinwoo Hwang, "Probing Nanoscale Structure of Disordered Materials Using 4-Dimensional Scanning TEM", *XXVII International Materials Research Congress*, Cancun, Mexico, August 19-24, 2018.
- R. A. Baker, R. Sakidja and A. Behzadan, "Immersive Virtual Reality (VR) Technologies for Introductory Physics Education". *33rd Showcase on Teaching and Learning* - August 15'18, MSU.
- D. Wilson, J. Gdovin, R. Sakidja, B. Jaegers, "Cross-Curricular Biophysics: Results of a Curricular Innovation Grant", *33rd Showcase on Teaching and Learning* - August 15, 2018, MSU.
- L. T. Kisson-Charles, T. Tran, J. Heiman, R. Sakidja, "Lemna minor: Response to nanoparticle exposure", *the Society of Wetland Scientists Annual Meeting*, 5/29 – 6/1, 2018 in Denver, CO.
- R. Sakidja, W-Y Ching and C. Zhou, "Multimodal Approach to Modeling Creep Deformation in Ni-base Superalloys", *2018 NETL Annual Review Meeting for Crosscutting Research*, Pittsburgh, PA, April 10th -12th, 2018.
- (Invited) "Mitigating crack nucleation in metal-ceramic nanolaminate composites", *Dept. of Physics Colloquium*, University of Missouri-Kansas City, December 1st, 2017.
- K. Evans, M. P. McKay and R. Sakidja, "Matrix in Carbonate Impact Breccias Comminution and Precipitation from Supercritical Water (SCW)?", Poster presentation at the *Geological Society of America (GSA) 129th Annual Meeting*, October 22-15, 2017 in Seattle, WA.

- R. Sakidja, P. Simanjuntak and C. Zhou, "Atomistic and Meso-scale Modeling on Deformation and Fracture Behavior of TiN-Al Nanolaminates", *MS&T 2017*, October 8-12, 2017, in Pittsburgh, PA.
- Md. Shafiqul Islam, P. Simanjuntak, S. Mitra and R. Sakidja, "DFT Study on the Li Mobility in Li-ion-based Solid-state Electrolytes", *2017 MRS Spring Meeting*, Apr. 17-21'17, Phoenix, AZ.
- (Invited) "Use of ab-initio molecular dynamics and data mining for design and synthesis of novel nanomaterials", *41st International Conference & Expo on Advanced Ceramics and Composites (ICACC 2017)*, January 22 - 27, 2017, Daytona Beach, FL.
- (Invited) "Atomistic-Based Modeling on Nanomaterials", *Dept. of Physics, Colloquium at the University of Arkansas*, September 23rd, 2016, Fayetteville, AR.
- P. Simanjuntak, R. Sakidja and C. Zhou, "Development of Many-body Potentials for Al-TiN Nanolayered Composites", at *Materials Science and Technology 2016*, Oct. 23-27, 2016, Salt Lake City, UT. R. Sakidja and Z. Leuty, "On the Oxidation Mechanisms of High-temperature Intermetallic MAX Phases", *MS&T 2016*, October 23-27, 2016, Salt Lake City, UT.
- R. Mayanovic, S. Dey, R. Sakidja, Z. Wang, M. Mandal, K. Landskron, "In-situ X-ray Scattering Studies of Mesoporous Materials under Extreme Conditions", *MS&T 2016*, Oct. 23-27'16, Salt Lake City, UT.
- R. Sakidja and Z. Leuty, "On the Thermal Characteristics and Alloying Design in Al₅Fe₂ Phase", *Symposium on Phase Stability, Diffusion Kinetics, and their Applications (PSDK-X), MS&T 2015*, October 4-8, 2015, Columbus, OH.
- R. Sakidja, N. Li, W-Y Ching, "Ab Initio Molecular Dynamics Study on the Early-Stage Oxidation Mechanism of MAX Phases", *Symposium on Corrosion and Oxidation of High Temperature Materials, MS&T 2015*, October 4-8, 2015, Columbus, OH.
- R. Sakidja, Q. Liu, Y. Gong, J. Z. Wu, "Atomistic Design and Synthesis in a Synchronous Growth of Bilayer Graphene", *Symposium on Controlled Synthesis, Processing, and Applications of Structural and Functional Nanomaterials, MS&T 2015*, October 4-8, 2015, Columbus, OH.
- D. R. Soden, R. Sakidja and K. Ghosh, "Bio Interactions Between Zinc-Oxide Nanorods and Adenosine Triphosphate", *Symposium on Surface Properties of Biomaterials, MS&T 2015*, October 4-8, 2015, Columbus, OH.
- (Invited) "Atomistic based Materials Modeling on Novel Carbon Complexes", at *Brewer Science (JVIC)*, March 5th, 2015, Springfield, MO.
- (Invited) "Designs in refractory metal-based silicides and aluminides for high-temperature coating applications", at *Intermetallics 2013*, Sept. 30-Oct. 4, 2013, Kloster Banz, Germany.
- (Invited) "Accelerating materials property discoveries for high-temperature structural applications through ab initio molecular dynamics simulations", at *10th Pacific Rim Conference on Ceramic and Glass Technology (PACRIM 10)*, Jun2 2-7, 2013, San Diego, CA.