

Research Interests

Material modification; material functionalization; materials in extreme conditions; microstructure evolution; defects; radiation-matter interactions; radiation effects; mechanical behavior; atomic dynamics; ion beam modification of materials; deformation mechanisms; atomistic modeling; functional materials; nuclear materials; ceramics; insulators; semiconductors; alloys; 2D materials; disordered materials; computational frameworks for materials science; machine-learning methods; force field development.

Professional experience

• Senior R&D Staff	2024 – present	Oak Ridge National Laboratory, TN, USA
• R&D Staff	2021 – 2024	Oak Ridge National Laboratory, TN, USA
• R&D Associate Atomistic Modeling	2016 – 2020	Oak Ridge National Laboratory, TN, USA
• Postdoctoral Research Associate	2014 – 2016	Oak Ridge National Laboratory, TN, USA
• Post-bachelor's Intern	02/2010 – 07/2010	National Hellenic Research Foundation, Athens, Greece

Education

- Ph.D. Physics, Queen Mary, University of London, UK, 2013
- B.Sc. Physics, 2009, National and Kapodistrian University of Athens, Greece

Publications Summary

Articles in Peer reviewed Journals:	56
Main author (1 st , last, corresponding):	30
Contributing author:	26
Book Chapters:	1
Technical report:	1

Google Scholar Metrics (Aug 2024)

Citations:	≥ 1500
h-index:	23

Presentations Summary

Total presentations:	60
Oral presentations in conferences:	27
Invited:	7
Oral presentations in seminars:	16
Invited:	4
Poster presentations:	17

Research Projects

1. Center for Nanophase Materials Sciences, Department of Energy, Basic Energy Sciences Scientific User Facilities Division, 2022-present
2. "Atomic Dynamics in Metallic and Other Liquids and Glasses," Co-Investigator, Department of Energy, Basic Energy Sciences, 2019-present.
3. "Computational Framework for Modeling Titanium Diboride Chemical Erosion by Plasma," Co-Investigator, ORNL Laboratory Directed Research and Development Program, 2024-2025
4. "Advanced Thermoelectric Conversion Technology for Radioisotope Thermoelectric Generators," Task Lead, ORNL Laboratory Directed Research and Development Program, 2022-2023
5. "Molecular dynamics simulations of precipitate evolution in lightweight alloys", Co-Investigator, Department of Energy, Vehicle Technologies Office, 2022-2023.
6. "The Material Plasma Exposure eXperiment (MPEX) Digital Twin," Co-Investigator, ORNL Laboratory Directed Research and Development Program, 2021-2022.

7. "Understanding and predicting radiation-resistant piezoelectric materials," Principal Investigator, ORNL Laboratory Directed Research and Development Program, 2019-2021.
8. "Multiscale Mechanical Properties and Alloy Design", Co-Investigator, Department of Energy, Basic Energy Sciences, 2019-2022.
9. "Machine Learning and Supercomputing to Predict Corrosion/Oxidation of High-Performance Valve Alloys," Co-Investigator, Department of Energy, Office of Energy, Efficiency Renewable Energy, 2020-2021.
10. "Electronic and Atomic Response of Ceramic Structures to Irradiation," Co-Investigator, Department of Energy, Office of Science, Basic Energy Sciences, 2016-2019.
11. "Energy Dissipation to Defect Evolution," Co-Investigator, Department of Energy, Office of Science, Basic Energy Sciences, Energy Frontier Research Center, 2016-2019.

Project Leadership

- "Understanding and predicting radiation-resistant piezoelectric materials," ORNL Laboratory Directed Research and Development Program, 2019-2021.
- Nuclear Science User Facilities (NSUF) Rapid Turnaround Experiment, Principal Investigator, "Post-irradiation Microstructure Characterization of Radiation-Tolerant Piezoelectric Materials," 2019-2021.
- Center for Nanophase Materials Sciences User Project, Principal Investigator, "Characterization of piezoelectric AlN, Sc-doped AlN and GaN materials after ion irradiation," 2020-2021.

Serving Leadership

- Vice Chair of the TMS Chemistry and Physics of Materials Committee, 2024-2026
- Appointed Member of ORNL Cultural Transformation Task Force, 2022-2023
- President of ORNL Women's Alliance Council, 2021- 2022
- Vice President of ORNL Women's Alliance Council, 2020 - 2021
- Chair of ORNL Women in Physical Sciences, 2018-2019

Serving Roles

- Mentor in *Greek Women in STEM*, 2021-present
- Mentor, Queen Mary University of London Alumni, 2013-present
- Board Member, ORNL Women's Alliance Council, 2023-2024
- Organizing Committee Member, ORNL Juneteenth Celebration, 2022, 2023
- Appointed Member, ORNL's Director's Search and Interview Committee, 2022
- Strategic Planning Committee Member, ORNL Physical Sciences, 2022, 2024
- Communications Chair, ORNL Women in Physical Sciences, 2017-2018
- Organizing Committee Member, ORNL Black History Month Celebration, 2018-2020
- Board Member, Women in Science and Engineering, Queen Mary, University of London, 2012-2013

Editorial Boards

- Advisor, JOM journal of TMS, 2021-2025
- Guest editor, Special Issue "Interface Engineering and Property Functionalization", JOM journal of TMS, under preparation, issue date August 2024
- Early Career Board Member, Nuclear Materials and Energy, 2022-present
- Guest Editor, Special Issue "Machine Learning and New Paradigms in Computational Materials Research," JOM journal of TMS, September 2022
- Energy Frontiers in Research Centers Newsletter, Editorial Board member, Department of Energy, 2016-2017

Conference Organization

1. TMS 2024 Symposium “Chemistry and Physics of Interfaces,” inaugural symposium, 2024
2. TMS 2024 Symposium “Computational Thermodynamics & Kinetics,” 2024
3. TMS 2023 Symposium “Computational Thermodynamics & Kinetics,” 2023
4. Oak Ridge National Laboratory Women’s Leadership Workshop, 2022
5. TMS 2022 Symposium “Computational Thermodynamics & Kinetics,” 2022
6. TMS 2021 Symposium “Computational Thermodynamics & Kinetics,” 2021
7. Oak Ridge National Laboratory Women’s Leadership Workshop, 2021
8. *Hermes* 2012 - London Summer School in Materials Simulation, 2012

Distinctions and Awards

- “Service Award - ORNL Women’s Alliance Council”, for improving diversity and inclusion, ensuring opportunities are available to network”, 2023.
- “Director’s Award,” for Outstanding Individual Accomplishment in Mission Support, UT-Battelle Awards Night, 2022.
- “One ORNL” Award, “for embodying the spirit of *One ORNL* by demonstrated efforts to create a unified laboratory community,” UT-Battelle Awards Night, 2022.
- “Outstanding Scholarly Output Team Award”, Science and Technology Category, UT-Battelle Awards Night, 2020.
- Best Team Effort Award, US Department of Energy, Office of Science, Basic Energy Sciences Contest *Intersection of Sound and Science Podcast*, Energy Frontiers Research Center-Hub-CMS Principal Investigators’ Meeting, Washington, DC, 2017.
- Best Student Poster Presentation Award, REI-17 Conference, University of Helsinki, Helsinki, 2013.
- Queen Mary, University of London, Postgraduate Travel Grant, 2013.
- Queen Mary, University of London, Postgraduate Travel Grant, 2012.
- SEPnet PhD Program Award, 2010-2013.

Professional Societies Memberships

- TMS 2016-present
 - a. Member, TMS Diversity, Equity, and Inclusion Committee, 2022-present
 - b. Member, TMS Emerging Professionals Committee, 2021-present
 - c. Member, TMS Computational Thermodynamics & Kinetics Committee, 2020-present
- Collaborative Computational Project 5 (CCP5) 2010-2013, 2020-present
- AnitaB.org Global Organization for Women Technologists, Sept 2021-2023
- American Ceramics Society (ACerS), 2014-2020
- Materials Research Society (MRS), 2012-2017
- Association for Iron & Steel Technology (AIST), 2016-2017

Presentations

Selected Oral Presentations at International Conferences

1. “Material modification: ion-matter interactions insights from atomistic modeling”, COSIRES - The 16th conference of Computer Simulation of Radiation Effects in Solids, Kingston, ON, Canada, June 2024, **Invited**
2. “Effects of Precipitate Size and Spacing on Deformation-induced fcc to bcc Phase Transformation,” TMS 2023, San Diego, CA, March 2023, **Invited**
3. “Electron-phonon Coupling Effects in Ion Irradiation of Metallic Systems,” TMS 2020, San Diego, CA, USA, 2020, **Invited**

4. "Stability of Al-Li-Ti-Sc-Mg High Entropy Alloys from Monte Carlo Simulations," TMS 2020, San Diego, CA, USA, 2020, **Invited**
5. "Effects of the electronic and nuclear energy loss in molecular dynamics simulations of irradiation," 42nd ICACC, Daytona, FL, USA, January 2018, **Invited**
6. "Molecular Dynamic Simulations of Synergistic Effects in Ion Track Formation," 39th ICACC, Daytona, FL, USA, January 2015, **Invited**

Selected Invited Seminars

1. "Whose Responsibility is DEIA in Stem After All?," Nuclear Engineering & Radiological Sciences Colloquium, University of Michigan, 2024, **Invited**
2. "Beam-matter interactions: Insights from atomistic modeling approaches," West Virginia University, February 2024, **Invited**
3. "Understanding and predicting radiation-matter interactions through atomistic modeling," Materials Science Department, Caltech, October 2023, **Invited**
4. "Molecular Dynamics Simulations of Materials at Extreme Conditions," National Hellenic Research Foundation, Athens, Greece, November 2021, **Invited**

Selected Poster Presentations

1. "Electron-phonon Coupling Effects in Ion Irradiation of Metallic Systems," TMS 2020, San Diego, CA, USA, March 2020
2. "Two-temperature Model Molecular Dynamics Simulations of irradiation of Ni and Ni-based alloys," 21st International Conference on Ion Beam Modifications in Materials, San Antonio TX, USA, June 2018
3. "Predictive Modeling of Synergistic Effects in Nanoscale Ion Track Formation," Multi-scale modelling of matter under extreme irradiation CECAM Workshop, Dublin, Ireland, June 2015
4. "Radiation Damage Modelling: Safe Encapsulation of Nuclear Waste," REI-17 Conference, University of Helsinki, Helsinki, July 2013, **Best Student Poster Presentation Award**
5. "Radiation Damage Modelling: Safe Encapsulation of Nuclear Waste and Fusion Applications," SEPnet Grand Challenge Conference, University of Southampton, UK, 2012

Book Chapter

1. R. E. Stoller, **E. Zarkadoula**, "Primary Radiation Damage Formation in Solids," Comprehensive Nuclear Materials (Second Edition), Konings R.J.M. and Stoller R.E., Elsevier, 2020.

Selected Refereed Journal Publications (* denotes corresponding author)

1. G. Velisa, D. Iancu, **E. Zarkadoula***, Y. Tong, Y. Zhang, W. J. Weber, "Ion velocity effect governs damage annealing process in defective KTaO₃," Journal of Physics D: Applied Physics, J. Phys. D: Appl. Phys. 57, 365303, 2024.
2. X. Han, R. Li, S. Pan, Y. Liu, C. Niu, M. L Crespillo, **E. Zarkadoula***, P. Liu, "Tailoring the Electronic Structures and Spectral Properties of ZnO with Irradiation Defects Generated Under Intense Electronic Excitation: A Combined Experimental and DFT Approach", Adv. Funct. Mater. 2405885, 2024.
3. X. Han, **E. Zarkadoula***, M. L. Crespillo, Q. Huang, S. Pan, C. Liu, M. Zhang, "Structural Damage and Recrystallization Response of Garnet Crystals to Intense Electronic Excitation," Adv. Funct. Mater. 2212853, 2023.

4. X. Han, **E. Zarkadoula***, Q. Huang, M. L. Crespillo, C. Liu, M. Zhang, X. Wang, P. Liu, "Nanostructures evolution assessment and spectroscopic properties modification induced by electronic energy loss in KTaO_3 crystal," *Mater. & Des.*, 223, 111248, 2022.
5. B. LaRiviere, P. Ramuhalli, F. K. Reed, P. C. Joshi, M. N. Ericson, T. Aytug, M. L. Crespillo, S. J. Zinkle, W. J. Weber, **E. Zarkadoula***, "Irradiation-induced Degradation of Surface Acoustic Wave Devices Fabricated on Bulk AlN," *Trans Device Mater Reliab.*, 2022.
6. Y. Osetsky, M.H. Du, G. Samolyuk, S. J. Zinkle, **E. Zarkadoula***, "Native and radiation induced point defects in AlN and Sc-doped AlN," *Phys. Rev. Mat.*, 6 (9), 094603, 2022.
7. **E. Zarkadoula***, Y. Yang, A. Borisevich, E. George, "Effects of precipitate size and spacing on deformation-induced fcc to bcc phase transformation," *Mater. Res. Lett.* 10 (9), 585-592, 2022.
8. **E. Zarkadoula***, Y. Shinohara, T. Egami, "X-ray free-electron laser heating of water at picosecond timescale," *Phys. Rev. Res.*, 4, 013022, 2022.
9. Y.C. Lin, C. Liu, Y. Yu, **E. Zarkadoula**, Y. Yoon, A. A. Puretzky, L. Liang, X. Kong, Y. Gu, A. Strasser, H. M. Meyer III, M. Lorenz, M. F. Chisholm, I. N. Ivanov, C. N. Rouleau, G. Duscher, K. Xiao, D. B. Geohegan, "Low Energy Implantation into Transition-Metal Dichalcogenide Monolayers to Form Janus Structures," *ACS nano*, 14 (4), 3896, 2020. **Outstanding Scholarly Output Team Award**
10. **E. Zarkadoula***, G. Samolyuk, W. J. Weber, "Effects of electron-phonon coupling and electronic thermal conductivity in high energy molecular dynamics simulations of irradiation cascades in nickel," *Comput. Mater. Sci.* 162, 156-161, 2019.
11. **E. Zarkadoula***, G. Samolyuk, W. J. Weber, "Effects of the electron-phonon coupling activation in collision cascades," *J. Nucl. Mater.*, 490, 317-322, 2017.
12. **E. Zarkadoula***, G. Samolyuk, H. Xue, H. Bei, and W. J. Weber, "Effects of two-temperature model on cascade evolution in Ni and NiFe," *Scripta Mater.*, 124, 6-10, 2016.
13. **E. Zarkadoula***, H. Xue, Y. Zhang, W. J. Weber, "Synergy of inelastic and elastic energy loss: Temperature effects and electronic stopping power dependence," *Scripta Mater.*, 110, 2-5, 2016.
14. **E. Zarkadoula***, O. Pakarinen, H. Xue, Y. Zhang, and W.J. Weber, "Predictive Modeling of Synergistic Effects in Nanoscale Ion Track Formation", *Phys. Chem. Chem. Phys.*, 17, 22538, 2015.
15. **E. Zarkadoula***, S. L. Daraszewicz, D. M. Duffy, M. Seaton, I. T. Todorov, M. T. Dove, K. Nordlund, and K. Trachenko "The nature of high-energy radiation damage in iron," *J. Phys.: Condens. Mat.*, 25, 125402 2013, **IoP Select**.