

Eva Zarkadoula, Ph.D. Physics
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Contact Information

Oak Ridge National Laboratory (ORNL)
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Research Interests

Material modification; material functionalization; materials in extreme conditions; material properties; microstructure alterations; defects; radiation-matter interactions; radiation effects; mechanical behavior; atomic dynamics; ion beam modification of materials; deformation mechanisms; fusion; atomistic modeling; functional materials; nuclear materials; ceramics; insulators; semiconductors; alloys; 2D materials; disordered materials; glasses; liquids; computational frameworks for materials science.

Professional experience

Senior R&D Staff, 2024 – present
Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, TN, USA.

R&D Staff, 2022 – 2024
Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, TN, USA.

R&D Staff, 2021 – 2022
Materials Science and Technology Division, Oak Ridge National Laboratory, TN, USA.

R&D Associate – Atomistic Modeling, 2016 – 2020
Materials Science and Technology Division, Oak Ridge National Laboratory, TN, USA.

Postdoctoral Research Associate, 2014 – 2016
Materials Science and Technology Division, Oak Ridge National Laboratory, TN, USA.

Post-bachelor's Project, Feb. 2010 – July 2010
Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece.

Education

Ph.D. Physics, 2013, Queen Mary, University of London, UK

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Thesis: Modelling of High-energy Radiation Damage in Materials relevant to Nuclear and Fusion Energy

B.Sc. Physics, 2009, National and Kapodistrian University of Athens, Athens, Greece (Level 5, according to the International Standard Classification of Education, ISCED), Grade: “Very Good”

Research Grants

1. “Atomic Dynamics in Metallic and Other Liquids and Glasses,” Co-Investigator, Department of Energy, Basic Energy Sciences, 2019 – present.
2. “Advanced Thermoelectric Conversion Technology for Radioisotope Thermoelectric Generators,” Task Lead, ORNL Laboratory Directed Research and Development Program, 2022-2023
3. “Molecular dynamics simulations of precipitate evolution in lightweight alloys” for the Powertrain Materials Core Program, Co-Investigator, Department of Energy, Vehicle Technologies Office, 2022 – 2023.
4. “The Material Plasma Exposure eXperiment (MPEX) Digital Twin,” Co-Investigator, ORNL Laboratory Directed Research and Development Program, 2021 –2022.
5. “Understanding and predicting radiation-resistant piezoelectric materials,” Principal Investigator, ORNL Laboratory Directed Research and Development Program, 2019-2021.
6. “Multiscale Mechanical Properties and Alloy Design”, Co-Investigator, Department of Energy, Basic Energy Sciences, 2019 – 2022.
7. “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.
8. “Electronic and Atomic Response of Ceramic Structures to Irradiation,” Co-Investigator, Department of Energy, Office of Science, Basic Energy Sciences, 2016 – 2019.
9. “Energy Dissipation to Defect Evolution,” Co-Investigator, Department of Energy, Office of Science, Basic Energy Sciences, Energy Frontier Research Center, 2016 – 2019.

Leadership Activities

Project Management

1. Project lead and manager– Principal investigator “Understanding and predicting radiation-resistant piezoelectric materials,” ORNL Laboratory Directed Research and Development Program, 2019-2021.
2. Project lead - Nuclear Science User Facilities (NSUF) Rapid Turnaround Experiment, Principal Investigator, “Post-irradiation Microstructure Characterization of Radiation-Tolerant Piezoelectric Materials,” 2019-2021.
3. Project lead - ORNL Center for Nanophase Materials Sciences (CNMS) User Project, Principal Investigator, “Characterization of piezoelectric AlN, Sc-doped AlN and GaN materials after ion irradiation,” 2020-2022.

Other Leadership Activities

1. President of ORNL Women's Alliance Council Employee Resource Group, June 2021-present
2. Appointed Member of ORNL Cultural Transformation Task Force, Jan. 2022-present
3. Chair of ORNL Women in Physical Sciences, 2018-2019

Editorial Boards

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

Symposium Organizing and Chairing

Organizing

1. The Minerals, Metals & Materials Society (TMS) 2024 Symposium "Chemistry and Physics of Interfaces," inaugural symposium, 2024
2. The Minerals, Metals & Materials Society (TMS) 2024 Symposium "Computational Thermodynamics & Kinetics," 2024
3. The Minerals, Metals & Materials Society (TMS) 2023 Symposium "Computational Thermodynamics & Kinetics," 2023
4. Oak Ridge National Laboratory Women's Leadership Workshop, 2022
5. The Minerals, Metals & Materials Society (TMS) 2022 Symposium "Computational Thermodynamics & Kinetics," 2022
6. The Minerals, Metals & Materials Society (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

Session Chair

1. TMS 2024 Chemistry and Physics of Interfaces – Grain Boundaries and Interfacial Line Defects, 2024

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2. TMS 2024 Chemistry and Physics of Interfaces – Surface and Interface Chemistry, 2024
3. TMS 2023 Computational Thermodynamics & Kinetics - Kinetics and Transport, 2023
4. TMS 2021 Computational Thermodynamics & Kinetics - Phase Stability I, 2021
5. TMS 2021 Computational Thermodynamics & Kinetics-Solidification, Additive Manufacturing/Ordering, Coarsening and Patterning, 2021.
6. TMS 2020 Computational Materials Science and Engineering of Materials in Nuclear Reactors — Multiscale Modeling II, 2020
7. “Atom by Atom Fabrication via Electron Beams and Scanning Probes”, Center for Nanophase Materials Sciences Oak Ridge National Laboratory, 2018

Distinctions and Awards

- “Service Award – ORNL Women’s Alliance Council. The award recognizes an individual who volunteers time, expertise, and resources within and across Oak Ridge National Laboratory communities with the goal of improving diversity and inclusion; an individual that ensures opportunities are available to network such that no woman feels isolated; or an individual that reaches out to mentor, collaborate, and nurture others,” 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.
- Department of Energy, Office of Science, Basic Energy Sciences Contest *Intersection of Sound and Science Podcast*, Best Team Effort Award, 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 Society Committees

- Elected Vice Chair of the Chemistry and Physics of Materials Committee of TMS (The Minerals, Metals & Materials Society), 2024-2026
- Member of TMS Diversity, Equity, and Inclusion Committee, 2022-present
- Member of TMS Emerging Professionals Committee Member, 2021-present
- Member of TMS Computational Thermodynamics & Kinetics Committee, 2020-present

Serving Roles / Memberships

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- Appointed Board Member for Culture & Climate, ORNL Women's Alliance Council Employee Resource Group, 2023-present
- Member of ORNL Juneteenth Celebration Organizing Committee, 2002 and 2023
- Appointed Member of ORNL's Director's Search and Interview Committee, August 2022-December 2022
- Appointed Member of ORNL Cultural Transformation Task Force, 2022-2024
- Member of ORNL Physical Sciences Strategic Planning Committee on Materials, Chemistry and Physics at the Extreme, May - August 2022
- Mentor in *Greek Women in STEM*, 2021-present
- President of ORNL's Women's Alliance Council, June 2021- Sept. 2022
- Vice President of ORNL Women's Alliance Council, 2020-2021
- Member of ORNL Women's Alliance Council, 2018-present
- Chair of ORNL Women in Physical Sciences, 2018-2019
- Communications Chair of ORNL Women in Physical Sciences, 2017-2018
- Member of ORNL Women in Physical Sciences ORNL Group, 2017-present
- Member of ORNL Black History Month Celebration Committee, 2018-2020
- Member of ORNL Early Career Professionals, 2017-2019
- Queen Mary University of London Alumni Mentor, 2013-present
- Board member of Women in Science and Engineering, Queen Mary, University of London, 2012-2013
- South-East Physics network (SEPnet) Member, 2010-2013

Professional Development

- Management Bootcamp, Oak Ridge National Laboratory, 03/2023
- Women's Leadership Workshop, Oak Ridge National Laboratory, 03/2022
- Grace Hopper Conference for Women Technologists, September 2021
- Women's Leadership Workshop, Oak Ridge National Laboratory, 03/2021
- Development course "Courageous Leaders' Summit," 01/2020
- Development course "Fostering a Positive Work Environment," 11/2019
- Development course "Effective Meetings," 07/2019
- Development course "Career Management," 06/2019
- Development course "Resiliency in the Workplace," 05/2019
- Development course "Your Science in a nutshell," 04/2019
- Women's Leadership Workshop, Oak Ridge National Laboratory, 03/2019
- Development course "7 Habits of Highly Effective Individuals," 02/2019
- ORNL Mentoring Program (by nomination only), 2018-2019
- Development course "Communication: The Art & Science of Connection," 10/2018
- Development course "Writing Federal Proposals," 08/2018
- Development course "Crucial Accountability," 07/2018
- Development course "Effective Scientific Writing Workshop," 01/2018

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- Development course “Crucial Conversations,” 12/2017

Outreach

- Panelist “Promoting Diversity and Overcoming Implicit Bias in Scientific User Facilities and User Groups”, CNMS User Meeting, 2023
- “What is a physicist doing in computational materials science?” Speaker Event for ORNL Interns and Staff, Eva Zarkadoula, ORNL Computing and Computational Sciences Directorate summer seminar, June 2023
- Panel member “Imposter Syndrome,” University of Tennessee, Knoxville, March 2022
- Partnership between ORNL’s Committee for Women and Women in Materials Science and Engineering at Georgia Institute of Technology, 2021
- APS March Meeting Physics Crossing Event, 03/2021
- Judge for Oral Presentations, Women in STEM Symposium, The University of Tennessee, Knoxville, 03/2019
- Poster Judge ASM International Students Poster Night, The University of Tennessee, Knoxville, 10/2018
- Poster Judge Women in STEM Symposium, UT Knoxville, 03/2018
- Poster Judge 6th ORPA Symposium, ORNL, 08/2018
- The Big Bang Fair, UK Scientists and Engineers Fair, Birmingham, UK, 2012
- Outreach for foundation year students, Queen Mary, University Of London, UK, 2011
- Outreach for primary school students, Queen Mary, University Of London, UK, 2011

Research in News Release

- News Release “Materials — Radiation-resistant sensors,” Published in ORNL News, Technology Networks, Technology Org, News wise, EurekAlert!, Bioengineer, 2022
- News Release “Process for ‘two-faced’ nanomaterials may aid energy, information tech,” Published in ORNL News; phys.org; newswise.com; scienmag.com; sciencenewsnet.in; nanowerk.com; eurekaalert.org; Science Daily; Nanotechnology Now; 7th Space; Primeur Magazine; Eurasia Review, 2020
- The Atlas of Science, “Predictive modeling of ion track formation during irradiation,” 2015

Presentations

Oral Presentations in Conferences

1. “Effects of Precipitate Size and Spacing on Deformation-induced fcc to bcc Phase Transformation,” *TMS2023*, San Diego, CA, March 2023, **Invited**
2. “X-ray Free-electron Laser Heating of Water at Picosecond Time Scale,” *TMS2023*, San Diego, CA, March 2023
3. “X-ray Free-electron Laser Heating of Water at Picosecond Time Scale,” *APS March Meeting 2023*, Las Vegas, NV, March 2023

4. "Atomistic Modeling of Phase Stability and Transformations due to the Presence of Precipitates in High and Medium Entropy Alloys," *TMS2022*, Anaheim, CA, USA, March 2022
5. "Electronic effects in atomistic modeling of radiation damage," *34th Annual Center for Simulational Physics Workshop*, University of Georgia, Athens, GA, USA, February 2021, **Invited**
6. "Electron-phonon Coupling Effects in Ion Irradiation of Metallic Systems," *TMS2020*, San Diego, CA, USA, 2020, Invited
7. "Stability of Al-Li-Ti-Sc-Mg High Entropy Alloys from Monte Carlo Simulations," *TMS2020*, San Diego, CA, USA, 2020, **Invited**
8. "Ion irradiation and microstructure alterations of ceramic materials," *MS&T18*, Columbus, OH, USA, October 2018
9. "Two-temperature model simulations of high energy cascades," *MS&T18*, Columbus, OH, USA, October 2018
10. "Modeling of ion irradiation induced microstructural alterations," *21st International Conference on Ion Beam Modifications in Materials*, San Antonio TX, USA, June 2018
11. "Effects of the electronic and nuclear energy loss in molecular dynamics simulations of irradiation," *42nd ICACC*, Daytona, FL, USA, January 2018, **Invited**
12. "Molecular Dynamics Simulations of Cascades: Effects of ion-electron interaction in irradiated alloys," Department of Energy, Office of Science, Basic Energy Sciences, Energy Frontiers Research Center PI Meeting, Washington DC, USA, July 2017
13. "Coupled effects of nuclear and electronic energy loss in ion irradiation," *MRS Fall Meeting*, Boston, MA, USA, November 2016
14. "Two-temperature model Molecular Dynamics Simulations of irradiation of Ni and Ni-based alloys," *MRS Fall Meeting*, Boston, MA, USA, November 2016
15. "Coupled effects of nuclear and electronic energy loss in ceramics under irradiation," *MS&T16*, Salt Lake City, UT, USA, October 2016
16. "Effects of the two-temperature model on cascade evolution in Ni and Ni-based alloys," *MS&T16*, Salt Lake City, UT, USA, October 2016
17. "Molecular Dynamic Simulations of Synergistic Effects in Ion Track Formation," *MS&T15*, Columbus, OH, USA, October 2015
18. "Molecular Dynamic Simulations of Synergistic Effects in Ion Track Formation," *39th ICACC*, Daytona, FL, USA, January 2015, **Invited**
19. "Molecular Dynamics Simulations of Ion Tracks," *MRS Fall Meeting*, Boston, MA, USA, November 2014
20. "High-energy Radiation Damage Modelling," *2nd Annual ORNL Postdoc Research Symposium*, Oak Ridge National Laboratory, TN, USA, July 2014
21. EMRS Spring Meeting, Strasbourg, France, May 2013
22. Thomas Young Centre Student Day, Queen Mary, University of London, UK, 2012
23. "Radiation Damage Modelling: Safe Encapsulation of Nuclear Waste and Fusion Applications," *Research Frontiers in Radioactive Waste Management*, University of Sheffield, UK, 2012

24. “Molecular Dynamics Simulations of High-energy Radiation Damage in Nuclear Power and Fusion Applications,” *MRS Spring Meeting*, San Francisco, CA, USA, April 2012
25. “Molecular dynamics simulations of high-energy radiation damage in nuclear and fusion Applications,” CCP5 Annual Meeting, University of Bath, UK, 2011
26. “Safe Encapsulation of Nuclear Waste and Operation of Future Fusion Reactors,” SEPnet Annual Regional Conference, UK, 2011

Oral Presentations in Seminars and Meetings

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. “Materials at Extreme Conditions: Insights from Atomistic Modeling”, ORNL Quantum and Energy Materials Seminar Series, April 2023
5. “Molecular Dynamics Simulations of Materials at Extreme Conditions,” Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, June 2022
6. “Molecular Dynamics Simulations of Materials at Extreme Conditions,” Theoretical and Physical Chemistry Institute Seminar, National Hellenic Research Foundation, Athens, Greece, November 2021, **Invited**
7. “Effects of electronic excitation in ion irradiation of metallic systems,” Energy Dissipation to Defect Evolution Energy Frontiers Research Center All-Hands Meeting, ORNL, TN, USA, June 2019
8. “Effects of electronic excitation in atomistic modelling of ion irradiation,” Materials Theory Group Seminar ORNL, TN, USA, December 2018
9. “Two-temperature Modeling of ion irradiation in metallic systems,” Energy Dissipation to Defect Evolution Energy Frontiers Research Center All-Hands Meeting, ORNL, TN, USA, September 2018
10. “Atomistic Modeling of Radiation Damage - Coupled Effects of Nuclear and Electronic Energy Loss,” ORNL Physical Sciences Directorate Seminar, ORNL, TN, USA, September 2018
11. “Coupled action of the nuclear and electronic energy loss in ion irradiation of Ni-based alloys,” Energy Dissipation to Defect Evolution Energy Frontiers Research Center All-Hands Meeting, ORNL, TN, USA, June 2017
12. “Electronic effects in high-energy cascades in Ni and Ni-based alloys,” Energy Dissipation to Defect Evolution Energy Frontiers Research Center All-Hands Meeting, ORNL, TN, USA, January 2016
13. “High-energy Radiation Damage in Safe Encapsulation of Nuclear Waste and Fusion Applications,” Materials Science and Technology Division, Group Seminar, Oak Ridge National Laboratory, TN, USA, March 2014
14. “Radiation damage modelling: safe encapsulation of nuclear waste and fusion applications,” HPC Materials Chemistry Consortium Meeting, University College London, UK, 2013

15. Centre for Condensed Matter and Materials Physics, Group Seminar, Queen Mary, University of London, UK, 2012
16. "Radiation damage effects in nuclear power and fusion applications," HPC Materials Chemistry Consortium Meeting, University College London, UK, 2011

Poster Presentations

1. "Electron-phonon Coupling Effects in Ion Irradiation of Metallic Systems," *TMS2020*, San Diego, CA, USA, March 2020
2. "Two-temperature model Molecular Dynamics Simulations of irradiation of Ni and Ni-based alloys," Structural Materials Workshop, ORNL, TN, USA, August 2019
3. "Electron-phonon Coupling Effects on Energy Dissipation and Damage Production in Ion Irradiation of Nickel and Nickel-based Alloys," Department of Energy, Office of Science, Basic Research Science Energy Frontiers Research Center PI Meeting, Washington DC, USA, July 2019
4. "Electronic effects in Atomistic Modeling of Radiation Damage," Physical Sciences Directorate Advisory Committee Meeting, ORNL, TN, USA, November 2018
5. "Effects of electronic excitation in ion irradiation of metallic systems," Energy Dissipation to Defect Evolution Energy Frontiers Research Center All-Hands Meeting, ORNL, TN, USA, June 2018
6. "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
7. "MD Modeling of Energy Dissipation in Collision Cascades in CSAs," Energy Dissipation to Defect Evolution Energy Frontiers Research Center All-Hands Meeting, ORNL, TN, USA, January 2017
8. "Electronic effects in high-energy cascades," Energy Dissipation to Defect Evolution Energy Frontiers Research Center All-Hands Meeting, ORNL, TN, USA, January 2016
9. 2015 Mechanical Behavior and Radiation Effects PI Meeting, US D.O.E., Washington DC, USA, 2015
10. "Predictive Modeling of Synergistic Effects in Nanoscale Ion Track Formation," 3rd Annual ORNL Postdoc Research Symposium, Oak Ridge National Laboratory, TN, USA, June 2015
11. "Predictive Modeling of Synergistic Effects in Nanoscale Ion Track Formation," Multi-scale modelling of matter under extreme irradiation CECAM Workshop, Dublin, Ireland, June 2015
12. "Radiation Damage Modelling: Safe Encapsulation of Nuclear Waste," Transformational Technologies in Molecular Simulations Summer School, Madison, WI, USA, 2014
13. "Radiation Damage Modelling: Safe Encapsulation of Nuclear Waste," REI-17 Conference, University of Helsinki, Helsinki, July 2013, **Best Student Poster Presentation Award**
14. "Radiation Damage Modelling: Safe Encapsulation of Nuclear Waste and Fusion Applications," MSSC2012, Ab Initio Modelling in Solid State Chemistry Workshop, Imperial College London, UK, 2012

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15. "Radiation Damage Modelling: Safe Encapsulation of Nuclear Waste and Fusion Applications," SEPnet Grand Challenge Conference, University of Southampton, UK, 2012
16. Departmental Poster Competition, Queen Mary, University of London, UK, 2012
17. Departmental Poster Competition, Queen Mary, University of London, UK, 2011