Hamdy Arkoub

Upcoming Postdoc at INL | Computational Nuclear Materials

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EDUCATION

The Pennsylvania State University 01/2022 – 07/2026

- **Ph.D.** in Nuclear Engineering (GPA 3.79/4.00)
  Thesis: *"Multiscale Insights into Molten FLiNaK Salt Corrosion Mechanisms in NiCr Alloys"*
  Funding: *US NSF-funded CAREER Award (No. 2340019)*

Minor: Computational Materials Doctoral Minor

Alexandria University 09/2016 – 06/2021

- **B.Sc.** in the Nuclear and Radiation Engineering (GPA 3.84/4.00)
  Thesis: *"Research Reactor Design and its Experimental Facilities Including Thermal Column"*

Ranking: 1st in class 2021, Excellence with Degree of Honor

RESEARCH EXPERIENCES

Idaho National Laboratory (INL) Starting 08/2026

Computational Mechanics and Materials Department

- **Postdoctoral Associate:** Conducting engineering-scale computational research for fusion energy applications using MOOSE-based multiphysics tools, with a focus on tritium transport and plasma-facing materials modeling.

The Pennsylvania State University (PSU) 01/2022 – present

Ph.D. Student, Nuclear Engineering

- **Research Assistant:** Conducted research in the Computational Nuclear Materials Group (CNMG) under Prof. Miaomiao Jin, developing multiscale modeling frameworks for materials behavior in extreme environments using DFT, potential development, MD simulations, and kMC methods.

- **Research Mentorship:** Mentored undergraduates and graduate students in applying Molecular Dynamics simulations to investigate molten salt chemistry and corrosion. Mentorship resulted in tangible outcomes, including co-authorships and Conference Presentations at the ANS.

- **Collaborations:** Granted access to **Idaho National Lab HPC** (till Sep 2027) to support collaborative research with the CMM Department to develop and scale multiscale modeling tools.

  Collaborated within Penn State (**PSU Mechanical Engineering, PSU Computational Sciences**) to develop reactive force fields and a first-principles DFT database for property screening and training-set generation.

Idaho National Laboratory (INL) 05/2025 – 08/2025

Summer Intern

- Joined the Computational Mechanics and Materials Group at INL, conducted computational modeling of chemical ordering effects in Ni-based alloys subjected to molten salt using DFT (VASP) and ReaxFF MD (LAMMPS) simulations (manuscript under review).
- Developed and scaled kinetic Monte Carlo model from scratch in C++ using INL HPC systems, implementing parallelization strategies for large-scale simulations to connect atomic-scale simulations with engineering-relevant degradation behavior.

JOURNAL PUPLICATONS

1. **Arkoub, Hamdy**, Jia-Hong Ke, and Miaomiao Jin. "Atomistic Mechanisms of Stress-Dependent Molten Salt Corrosion in NiCr Alloys." *ACS Omega 030554 (2026).* *[DOI]*

2. **Arkoub, Hamdy**, Jia-Hong Ke, Kaustubh Bawane, and Miaomiao Jin. "Percolating Corrosion Pathways of Chemically Ordered NiCr Alloys in Molten Salts." *Corrosion Science 269 113960* (2026). *[DOI]*

3. **Arkoub, Hamdy**, Daniel Flynn, Adri CT van Duin, and Miaomiao Jin. "Surface Orientation-Dependent Corrosion Behavior of NiCr Alloys in Molten FLiNaK Salt." *ACS Applied Materials & Interfaces* 17(26):38708 (2025). *[DOI]*

4. **Arkoub, Hamdy**, and Miaomiao Jin. "First-principles investigation of grain boundary effects on fluorine-induced initial corrosion of NiCr alloys." *Computational Materials Science* 255 (2025): 113903. *[DOI]*

5. **Arkoub, Hamdy**, Swarit Dwivedi, Adri CT van Duin, and Miaomiao Jin. "A reactive force field approach to modeling corrosion of NiCr alloys in molten FLiNaK salts." *Applied Surface Science* (2024): 159627. *[DOI]*

6. **Arkoub Hamdy**, and Miaomiao Jin. "Impact of chemical short-range order on radiation damage in Fe-Ni-Cr alloys." *Scripta Materialia 229* (2023): 115373. *[DOI]*

In Progress:

7. Farshid Reza, **Arkoub, Hamdy**, Alexander Hauck, Adri CT van Duin, Miaomiao Jin. "Electric-field effects on defect migration energetics in GaN." arXiv preprint arXiv:2607.01160 (2026). (Under review: *Physical Review B*) *[DOI]*

8. Sadia Khan, **Arkoub, Hamdy**, and Miaomiao Jin. "Atomistic mechanism of corrosion-induced grain boundary migration in NiCr alloys in molten FLiNaK." arXiv preprint arXiv:2607.16167 (2026) (Submitted: *npj Materials Degradation*) *[DOI]*

9. **Arkoub, Hamdy**, Jia-Hong Ke, Nathan Bieberdorf, Miaomiao Jin. "Composition-Dependent Dealloying Pathways in Molten Salt Corrosion" *(Ongoing manuscript)*

PRESENTATIONS

- *"Kinetic Monte Carlo Modeling of Molten Salt Dealloying,"* Hamdy Arkoub, Jia-Hong Ke, Nathan Bieberdorf, Miaomiao Jin, **MS&T 2026 Annual Meeting & Exhibition** (Accepted)

- *"Multiscale Atomistic Modeling of Molten Salt Corrosion in NiCr Alloy,"* Hamdy Arkoub, Daniel Flynn, Swarit Dwivedi, Jia-Hong Ke, Kaustubh Bawane, Adri van Duin, Mia Jin, **PSU College of Engineering Research Symposium (CERS) 2026**

- *"Atomistic Insights into the Roles of Mechanical Strain and Chemical Ordering on Molten FLiNaK Salt Corrosion of NiCr Alloys,"* Hamdy Arkoub, Jia-Hong Ke, Kaustubh Bawane, Mia Jin, **TMS 2026 Annual Meeting & Exhibition**

- *"Multi-Scale Computational Modeling of Molten Salt Corrosion in NiCr Alloy,"* Hamdy Arkoub, Daniel Flynn, Swarit Dwivedi, Jia-Hong Ke, Kaustubh Bawane, Adri van Duin, Mia Jin, **TMS 2026 Annual Meeting & Exhibition**

- *"Revealing the Hidden Drivers of Molten Salt Corrosion,"* Hamdy Arkoub, Daniel Flynn, Swarit Dwivedi, Jia-Hong Ke, Adri van Duin, Mia Jin, **PSU Materials Day 2025**

- *"Orientation-Assisted Corrosion of NiCr Alloys in Molten FLiNaK Salt Using ReaxFF Molecular Dynamics,"* Hamdy Arkoub, Daniel Flynn, Adri van Duin, Mia Jin, **TMS 2025 Annual Meeting & Exhibition**

- *"Atomistic Insights into the Initial Corrosion Behavior of NiCr Alloys in Molten FLiNaK Salt,"* Hamdy Arkoub, Swarit Dwivedi, Adri van Duin, Mia Jin, **MS&T 2024 Annual Meeting & Exhibition**

- "A Reactive Force Field Approach to Modeling Corrosion of NiCr Alloys in Molten FLiNaK Salts." Hamdy Arkoub, Swarit Dwivedi, Adri van Duin, Mia Jin, **MS&T 2023 Annual Meeting & Exhibition**

- *"Investigate the Implications of Stacking Fault Energy on Radiation Damage and Deformation Behaviors of Fe-Ni-Cr Alloys,"* Hamdy Arkoub, Mia Jin, **MS&T 2022 Annual Meeting & Exhibition**

- *A Comprehensive Approach Towards Addressing Issues on High Level Waste Management Plan in the Republic of Korea,"* Jaewon Chung, Hamdy Arkoub, Woei Jer Ng, Naura Qotrunnada, **NEREC 2020 Conference on Nuclear Nonproliferation**

HONORS & AWARDS

Graduate Student, Penn State University

- **Best Poster Award** at the 2025 Penn State Nuclear Engineering Grad Day 09/2025
- **Vice Provost and Dean of Graduate School Student Persistence Scholarship**, awarded annually to a grad student across the entire university. 06/2025
- **Pitch your GEN IV Research Finalist worldwide**, invited by the Generation IV International Forum to present my research [YouTube Video]. 05/2025
- **Tau Beta Pi, the engineering honor society recognition,** for being in the top 1/8th of the class of engineering students. 10/2022

Undergraduate Student, Alexandria University

- **Mohamed Sawan Top Student Prize,** for graduating first in Class 2021 09/2021
- **Aly Mortada Award**, for the highest GPA in junior year, (3.92/4.0) 09/2020
- **Mohamed Elmaghrabi Award**, for the highest GPA in the second year, (3.95/4.0) 10/2019
- **Abdelhamid Elfaham Award**, for the highest GPA in freshman year, (4.0/4.0) 10/2018

MEMBERSHIPS

- **Postdoctoral Association at INL** 08/2026 – present
- **TMS Nuclear Materials Committe** 08/2025 – present
- **Institute of Nuclear Materials Management (INMM)** at Penn State 04/2024 – 05/2026
- **Material Advantage** 07/2022 – 10/2024

COMPUTER SKILLS

Programming Languages:
- Python (6+ years): workflows, HPC automation, ML (PyTorch, scikit-learn)
- C++(2+ years): parallelization concepts, kinetic Monte Carlo (kMC) modeling

Density Functional Theory (DFT):
- VASP and Quantum ESPRESSO (5+ years): interface energetics, PDOS
- Post-processing: VESTA, VMD (charge density, electron difference maps)

Molecular Dynamics (MD):
- LAMMPS (5+ years): large-scale MD, workflows, trajectory analysis, interfaces
- AMS (3+ years): reactive MD simulations, force-field development
- Analysis: OVITO, Atomsk, Packmol, custom Python scripts

Kinetic Monte Carlo (kMC):
- SPPARKS and custom C++/Python implementations: microstructure evolution

HPC Systems:
- Job scheduling & workflows: SLURM, PBS
- Clusters: Penn State RC (4+ years), Idaho National Laboratory HPC (1+ year)