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Opportunity Title: Artificial (Super) Intelligence, Chemistry, and Chemical Engineering
Opportunity Reference Code: ARL-WS-20261021-F1

Organization DEVCOM Army Research Laboratory

Reference Code ARL-WS-20261021-F1

How to Apply Applications must be submitted in Zintellect.

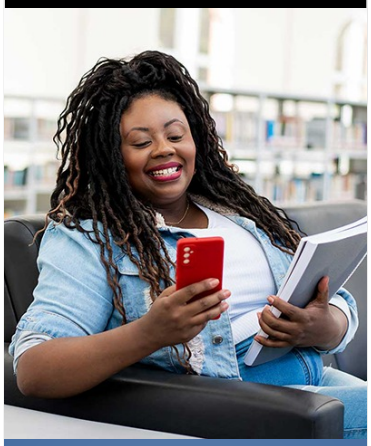
A complete application includes:

1. **Curriculum Vitae or Resume**
   - List relevant coursework and lab experience as well as all papers, presentations, or publications you may have authored or co-authored. Include any reprints or abstracts if they are available.
2. **Three References Forms**
   - An email with a link to the reference form will be available in Zintellect to the applicant upon completion of the on-line application. Please send this email to persons you have selected to complete a reference.
   - References should be from persons familiar with your educational and professional qualifications (include your thesis or dissertation advisor, if applicable)
3. **Transcripts**
   - Transcript verifying receipt of degree or current enrollment in an undergraduate or graduate program at an accredited university or technical institute. Student/unofficial copy is acceptable
4. **Research Proposal**
   - Research topic should relate to a specific opportunity at ARL
   - The objective of the research topic should be clear and have a defined outcome
   - Explain the direction you plan to pursue
   - Include expected period for completing the study
   - Include a brief background such as preparation and motivation for the research
   - References of published efforts may be used to improve the proposal

Description Postdoctoral research opportunity to design and build reactor models, chemical kinetics models, process models, and also perform fundamental research in artificial intelligence or machine learning methods for energetic materials. Research involves modeling of highly exothermic chemistry in various types of reactors at operational conditions. Research will involve creation of both traditional chemical engineering models, and Bayesian models or machine-learned models for reactors and process optimization. In addition to the reactor modeling, this fellowship offers freedom to pursue new ideas in AI/ML for energetic materials research in collaboration with a variety of institutions (including major R1 universities). Research products will include both traditional academic open literature publications and nonpublic technical reports. The postdoctoral researcher will have the opportunity to travel and give presentations at both traditional academic meetings and other nonpublic meetings.

DEVCOM ARMY RESEARCH LABORATORY

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Appointment will be Full-Time. One-year initial appointment with expectation for renewal to year two. Year three is dependent on performance and available funding.

ARL Advisor:
Brian Barnes
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About Army Research Directorate (ARD)

ARL's Army Research Directorate (ARD) focuses on exploiting concept development, discovery, technology development, and transition of the most promising disruptive science and technology to deliver to the Army fundamentally advantageous science-based capabilities through laboratory's 11 research competencies. This intramural research directorate also manages the laboratory's essential research programs, which are flagship research efforts focused on delivering defined outcomes.

About Weapon Sciences (WS)

Internal, transitional, and external ballistics; launch, flight, control, and navigation of guided weapons and aerial systems; development of novel weapon concepts.

You will be performing research with the:
Multiscale Reactive Modeling Team
Detonation Science and Modeling Branch
U.S. Army Combat Capabilities Development Command Army Research Laboratory

About Army Research Laboratory Research Associateship Program (ARL-RAP)

The Army Research Laboratory Research Associateship Program (ARL-RAP) is designed to significantly increase the involvement of creative and highly trained scientists and engineers from academia and industry in scientific and technical areas of interest and relevance to the Army. Scientists and Engineers at the CCDC Army Research Laboratory (ARL) help shape and execute the Army's program for meeting the challenge of developing technologies that will support Army forces in meeting future operational needs by pursuing scientific research and technological developments in diverse fields such as: applied mathematics, atmospheric characterization, simulation and human modeling, digital/optical signal processing, nanotechnology, material science and technology, multifunctional technology, combustion processes, propulsion and flight physics, communication and networking, and computational and information sciences.

Questions about this opportunity? Please email ARLFellowship@orau.org

Qualifications Security restriction: This fellowship requires a U.S. citizen able to pass a

background check.

Requirements: A Ph.D. in chemical engineering, chemistry, materials engineering, mechanical engineering, materials science, computer science, or artificial intelligence engineering. If you have equivalent skills that meet the project needs, but a different degree, please consider applying.

Desired knowledge, skills, and abilities:
- Experience with Python programming, including the chemistry module “rdkit” and the scientific Python stack.
- Bachelor's or above level knowledge of chemical reactor modeling (e.g. CSTRs, PFRs, Semi-batch reactors).
- Bachelor’s or above level knowledge of chemical kinetics.
- Experience developing artificial intelligence or machine learning models in python.
- Experience with version control using git, and Linux or macOS shells (bash or zsh).
- Interest in using AI coding agents (e.g. harnessed GPT-5.4) to assist or review scientific software development.
- Bachelor’s or above level knowledge of organic chemistry and thermodynamics.
- Experience modeling transport phenomena.
- Experience with HPC queueing systems such as PBS or Slurm.
- Experience with relational databases or data tooling such as Parquet/Arrow.
- Experience in multiphysics or process modeling simulations using software such as COMSOL Multiphysics, Cantera, ASPEN, or other packages used to create digital twins for chemical engineering applications.

It is not expected that the successful applicant will possess all of the above; if you have some but not all of the skills and an interest in the fellowship, please apply or contact the POC for further information. Applications will be accepted until the fellowship is filled.

Point of Contact ARL-RAP

Eligibility Requirements

- **Citizenship:** U.S. Citizen Only
- **Degree:** Master's Degree or Doctoral Degree.
- **Academic Level(s):** Master’s Degree 7+ years (Senior Fellow), Doctoral Degree (Postdoctoral Fellow), Doctoral Degree 5+ years (Senior Fellow), or Faculty.
- **Discipline(s):**
  - **Chemistry and Materials Sciences** (12 👁)
  - **Communications and Graphics Design** (2 👁)
  - **Computer, Information, and Data Sciences** (17 👁)
  - **Earth and Geosciences** (21 👁)
  - **Engineering** (29 👁)
  - **Environmental and Marine Sciences** (14 👁)
  - **Life Health and Medical Sciences** (51 👁)

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- **Mathematics and Statistics** (11 👁)
- **Physics** (16 👁)
- **Science & Engineering-related** (2 👁)
- **Social and Behavioral Sciences** (29 👁)