

Postdoctoral Opening in Data Science and Computational Chemistry for Electrolyte Discovery

The [Amanchukwu Laboratory](#) at the University of Chicago invites applications for a postdoctoral position focusing on computational chemistry and data science. The project involves the use of machine learning (ML) algorithms for electrolyte discovery and the use of quantum chemical tools such as molecular dynamics and/or density functional theory (DFT) to probe ion transport and generate features for the ML models. *The ideal candidate is a computational chemist with machine learning experience interested in diving into the world of electrolytes, batteries, and electrochemistry.* There are numerous opportunities for the candidate to engage with collaborators at the University of Chicago and at Argonne National Lab. The duration of the appointment is one year with a flexible start date. Reappointment will be possible, but dependent on performance and availability of funds.

Application details: Please send an electronic copy of your CV, brief (1 page) statement of research interests and future career goals. Use the Subject Line “Postdoc Application Data Science.” Email chibueze@uchicago.edu

Ideal skills: Applicant should have prior experience in data science/machine learning (e.g., scikit-learn) and experience in molecular dynamics and/or density functional theory. Must be proficient in Python and at least one of the following computational chemistry tools (e.g., GROMACS, NWChem, Gaussian, VASP etc.). No prior experience in batteries, electrolytes, or sustainability is required.

Location: On-site at the University of Chicago (desired). However, can also be remote.

Ideal applicants: Applicants conversant in computational chemistry and data science (machine learning etc.) Applicant must be self-motivated, driven and must be interested in working with students (undergraduates and graduate students). Applicant may be expected to work with the PI and contribute to grant applications. Applicant will be expected to apply to eligible fellowship opportunities that can also support their work.

The Amanchukwu Lab designs novel electrolytes with the focus of correlating bulk solvation properties to electrochemical phenomena in batteries and electrocatalysis. The PI holds a joint appointment at the University of Chicago and at Argonne National Laboratory. The Pritzker School of Molecular Engineering at the University of Chicago is the first school of molecular engineering in the United States with a focus on changing the way engineering challenges are solved. Furthermore, Chicago is a world class city.

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