

Candidate Information

Position:	Research Fellow in Machine Learning for Computational Water Treatment
School/Department:	Centre for Quantum Materials and Technology (CQMT)
Reference:	23/111452
Closing Date:	Monday 11 December 2023
Salary:	£37,841 per annum
Anticipated Interview Date:	Monday 8 January 2024
Duration:	Fixed term for 24 months

JOB PURPOSE:

To be a highly productive, ambitious and collaborative member of the research team working on the EPSRC New Investigator Award "Machine Learning for Computational Water Treatment" assisting in the development of research proposals and the planning and delivery of the research activity specifically running molecular dynamics simulations and developing machine learning models for the ability of materials to remove endocrine disruptors from drinking water.

The post is a critical role, and as such, successful applicants will have responsibilities in independent research, supervision, planning, day to day lab management, collaborations, and outreach.

MAJOR DUTIES:

1. Undertake research under supervision as a member of the "Machine Learning for Computational Water Treatment" research team.
2. Design, develop and refine research using a range of atomistic simulation techniques including molecular dynamics and machine learning.
3. Carry out analyses, critical evaluations, and interpretations of simulation data and the literature using methodologies and other techniques appropriate to area of research, as above.
4. Produce high quality research outputs consistent with project aims and commensurate with career stage. This will include collaborating and co-authoring with PI and project team (as appropriate) on outputs.
5. In consultation with the project team, promote research milestones and outputs at national and international conferences.
6. Assist grant holder in the preparation of funding proposals and applications to external bodies.
7. Carry out occasional educational supervision, demonstrating or lecturing duties within the post holder's area of expertise and under the direct guidance of a member of academic staff.
8. Undertake supplementary duties relevant to the success of the project including administrative duties and additional training and development activities as required.

ESSENTIAL CRITERIA:

1. Normally have or be about to obtain a PhD in chemistry, physics, materials science or a related discipline.
2. Specific relevant research experience in computer simulation including:
 - Undertaking research including atomistic simulations and/or machine learning.
 - A proven track record in carrying out computer simulations and critically analysing and interpreting their results.
 - Working effectively as part of a research team in the development and promotion of the research theme.
3. Strong publication record commensurate with stage of career.
4. Ability to contribute to broader management and administrative processes.
5. Practical problem solving skills, independence of thought and initiative.
6. Ability to assess and organise resources.
7. Ability to communicate complex information in English effectively in oral and written format.
8. Ability to build relationships to develop internal and external networks.
9. Commitment to continuous professional development.

DESIRABLE CRITERIA:

1. Experience with using a range of (empirical/machine learning) forcefields for atomistic simulation.
2. Experience in forcefield modification/development.
3. Contribute to the School's outreach programme by links with industry, community groups etc.