

Job Title:	Research associate in development of computational methods for NanoElectrochemistry
Department/Division/Faculty:	Faculty of Natural Sciences, Department of Chemistry
Campus location:	White City
Job Family/Level:	Research Family, Research Associate Level
Responsible to:	Dr. Clotilde S. Cucinota (EPSRC Fellow, Department of Chemistry)
Key Working Relationships (internal):	Research Staff, PhD, MRes and Undergraduate students within the Cucinotta's group, other members of the Department of Chemistry
Key Working Relationships (external):	Dr. Ivan Rungger, Senior Research Scientist, NPL (UK) and Dr. Marcella Iannuzzi, Privat Dozentin Doctor, UZH (CH)
Contract type:	Fixed term, 24 months

Purpose of the Post

A postdoctoral position is available in the Computational NanoElectrochemistry group at Imperial College London, in collaboration with the National Physics Laboratory (NPL), UK and University of Zurich (UZH), Switzerland, CH.

The project <https://gow.epsrc.ukri.org/NGBOViewGrant.aspx?GrantRef=EP/P033555/1> is on developing and applying new theoretical methodologies to enable the grand canonical modelling of electrochemical (EC) transformation under operating conditions, i.e. under the presence of an electric current and an applied potential (WP1). The developed tools will be used by the team to study (i) fundamental electro-catalytic phenomena at electrified interfaces (WP2), as found in corrosion and water splitting and (ii) current and bias induced effects at nanointerfaces such as electromigration, electromechanics and redox/resistive switching (WP3).

This role will develop a stationary non-equilibrium reformulation of Density Functional Theory (DFT) based molecular dynamics (MD), where the functional embed information on electronic currents and applied bias in addition to the equilibrium electron density. A key task will be the implementation of an interface between two very popular codes, Smeagol (for electron transport) (Smeagol) and CP2K (for DFT). The aim is to enable the calculation of current and bias induced forces, which will be used to perform grand canonical MD under bias. You will be interacting with the main developers of Smeagol and CP2K codes at NPL and UZH.

You will have the main responsibility for developing WP1. In addition, you will support the other members of the team in the use of the developed software within their sub-projects (WP2 and WP3).

Key Responsibilities

- To set up the simulation environment to perform molecular dynamics under bias by interfacing the Smeagol and CP2K codes, in collaboration with the lead investigator, the main developers of these codes and with the support of CPUK-UK network.
- To support the lead investigator in the supervision of the other members of the team.
- To take initiative in the planning of the research, in collaboration with and within the research area agreed with the lead investigator. Depending on your interests, after the first implementation phase the project you will have the opportunity agree with the PI to work on more theoretical, computational or applicative aspects of non-equilibrium grand canonical molecular dynamics.
- To maintain accurate and complete records of all progress communicate your research periodically to the group and the PI.
- To provide guidance to other team members and students on the application of the newly developed methodologies
- To support the PI in the instruction of PhD, MRes and project students as agreed
- To supervise practical work and advise students on methodologies

- To travel, as required, for meetings with actual and potential collaborators, and to attend conferences
- To write regular (monthly) internal reports as well as more detailed quarterly reports and other ad hoc reports as requested by the principal investigator
- To prepare material for presentation in oral and poster formats
- To present findings to colleagues and at workshops/conferences
- To draft publications and prepare them for submission to refereed journals
- To submit publications to refereed journals
- To contribute to writing bids for research grants
- To develop contacts and research collaborations within the College and the wider community
- To promote the reputation of the Group, the Department and the College

Other Duties

- To undertake appropriate administration tasks as agreed with the principal investigator
- To attend relevant meetings
- To be responsible for ensuring that research output is accurate, up-to-date and complete
- Any other duties commensurate with the grade of the post as directed by the principal investigator

Person Specification

Requirements	Essential (E)/ Desirable (D)
Candidates/post holders will be expected to demonstrate the following	
Education	
PhD (or equivalent) in Physics, Chemistry or related discipline.	E
Experience and Knowledge	
Experience of parallel programming in Fortran/C++ for distributed computing (e.g. MPI) and/or shared memory (e.g. OpenMP) architectures for scientific software development	E
Experience of writing and/or using scientific modelling codes in a technical or research environment	E
A strong background in fundamental physics and/or chemistry, electronic structure theory and/or modern computational approaches to materials.	E
Knowledge and experience in applying or developing DFT	D
Knowledge and experience in applying or developing methods for molecular dynamics	D
Knowledge and experience in applying or developing methods for molecular electronics	D
Knowledge and experience in applying or developing methods for reconstructing potential/free energy surfaces	D
Previous experience at postdoctoral level	D
Skills, Abilities and Personal Attributes	
Excellent written and verbal communication skills	E
Ability to support the PI in directing the work of a small research team and motivate others to produce a high standard of work	E
Ability to develop and apply new concepts	E
Creative approach to problem-solving	E
Ability to organise own work with minimal supervision	E
Ability to prioritise own work in response to deadlines	E
Willingness to work as part of a team and to be open-minded and cooperative	E
Flexible attitude towards work	E
Discipline and regard for confidentiality and security at all times	E
Willingness to undertake training for the role	E
Willingness to travel both within the United Kingdom and abroad to conduct research and attend conferences	E

Please note that job descriptions cannot be exhaustive and the post-holder may be required to undertake other duties, which are broadly in line with the above key responsibilities.

Imperial College is committed to equality of opportunity and to eliminating discrimination. All employees are expected to follow the [7 Imperial Expectations](#) detailed below:

- 1) Champion a positive approach to change and opportunity
- 2) Encourage inclusive participation and eliminate discrimination
- 3) Communicate regularly and effectively within and across teams
- 4) Consider the thoughts and expectations of others
- 5) Deliver positive outcomes
- 6) Develop and grow skills and expertise
- 7) Work in a planned and managed way

Employees are also required to comply with all College policies and regulations paying special attention to:

- Confidentiality
- Conflict of Interest
- Data Protection
- Equal Opportunities
- Financial Regulations
- Health and Safety
- Information Technology
- Smoking
- Private Engagements and Register of Interests

They must also undertake specific training and assume responsibility for safety relevant to specific roles, as set out on the [College Website Health and Safety Structure and Responsibilities](#) page.

The College is a proud signatory to the San-Francisco Declaration on Research Assessment (DORA), which means that in hiring and promotion decisions, we evaluate applicants on the quality of their work, not the journal impact factor where it is published. For more information, see <https://www.imperial.ac.uk/research-and-innovation/about-imperial-research/research-evaluation/>

The College believes that the use of animals in research is vital to improve human and animal health and welfare. Animals may only be used in research programmes where their use is shown to be necessary for developing new treatments and making medical advances. Imperial is committed to ensuring that, in cases where this research is deemed essential, all animals in the College's care are treated with full respect, and that all staff involved with this work show due consideration at every level.

<http://www.imperial.ac.uk/research-and-innovation/about-imperial-research/research-integrity/animal-research/>

Committed to equality and valuing diversity, we are an Athena SWAN Silver Award winner, a Stonewall Diversity Champion, a Disability Confident Employer and work in partnership with GIRES to promote respect for trans people.