University of Nottingham
UK | CHINA | MALAYSIA

Role profile

Job title	Research Associate/ Fellow in Theoretical Modelling of Heterogeneous Catalysis	Job family and level	Research and Teaching Level 4/4a+
School/ Department	Chemistry	Location	Chemistry Building, University Park, Nottingham, NG7 2RD

Purpose of role

Metal Atoms on Surfaces and Interfaces (MASI) is a large-scale multidisciplinary project spearheaded by four UK universities (Nottingham, Cardiff, Cambridge, and Birmingham) simultaneously addressing two grand challenges: sustainable use of metals and low-carbon technologies. The project is motivated by natural (limited resource of critical metals) and anthropogenic (overpopulation, global warming) threats rapidly beginning to impact society. The multidisciplinary holistic research methodology of MASI will stimulate innovation across different sectors and accelerate the translation of fundamental discoveries for clean technologies, thus realising the Productive Nation, Resilient Nation and Healthy Nation EPSRC ambitions.

The project consists of four interconnected Themes addressing the fundamental aspects of metal nanocluster formation (A), metal-support interactions (B), imaging & analysis of nanocatalysts in action (C) and harnessing their catalytic/electrocatalytic properties in key reactions, including CO_2 electroreduction and hydrogen generation by electrolysis (D), funded by the EPSRC Programme Grant for a period of five years. For more information, please visit www.MASI.ac.uk. We seek to appoint a Research Fellow to join the multidisciplinary MASI team, who will bring expertise in computational modelling for heterogeneous catalysts, including interactions and bonding of small molecules (e.g. CO_2, H_2, N_2) with metal nanoclusters and chemical reactions on metals and hybrid interfaces. The Research Fellow will become part of the Computational Materials Science group, led by Prof. Elena Besley (https://ebesley.chem.nottingham.ac.uk/).

The Research Fellow will be appointed for one year and is expected to take leadership in developing novel theoretical approaches to study interfacial chemical reactions and transport phenomena focusing on catalytic activity and selectivity of different metal nanoclusters in a range of chemical reactions. The Fellow will work in close collaboration with other theoretical and experimental scientists in the MASI research team to develop comprehensive multiscale models and computational approaches to address the fundamental challenges of nanocatalysis.

	Main responsibilities (Primary accountabilities and responsibilities expected to fulfil the role)	**% time per year**
1	Develop ab initio methods to study catalytic activity and selectivity of metal nanoclusters in a range of chemical reactions	40 %
2	Develop models of chemical kinetics of magnetron sputtering	15 %
3	Apply the models of chemical kinetics to study heterogeneous catalysis	15 %

4	Contribute to and actively participate in the design and execution of research to address defined problems, through collaboration with scientists in the MASI multidisciplinary team environment to accomplish research goals.	15%
5	Pursue independent but complementary research interests and interact with a broad spectrum of scientists internally and externally to the MASI project.	5%
6	Document research; publish papers in peer-reviewed journals, and present results within the community and at conferences.	5 %
7	Perform other duties as assigned.	5 %

Person specification

	Essential	Desirable
Skills	Skills in the application of first-principles simulations to heterogeneous catalysis and complex reactive interfaces involving metal nanoclusters. Proven ability to innovate using a range of *ab initio* codes, data acquisition, and data analysis methodologies. Ability to deliver high quality original research, as evidenced by a strong track record of publications in peer-reviewed journals, commensurate with career stage. Excellent verbal and written communication skills, as evidenced by presentations at seminars, conferences and/or teaching lectures. Initiative and interpersonal skills with desire and ability to work in a collaborative, multidisciplinary team environment.	Multiscale integration of first-principles calculations within kinetic models, including kinetic Monte Carlo, microkinetic models, Transition State Theory (TST) and coarse-grained approaches. Application of machine learning methods to problems of relevance in materials science. Methods for free energy sampling, global minimisation, and/or complex optimisation. Skills in writing research proposals.
Knowledge and experience	Knowledge of the concepts of density functional theory and first-principles molecular dynamics simulations. Track record in collaborative multi- and interdisciplinary research.	Experience in supervising research students. Experience of public outreach activities.
Qualifications, certification and training (relevant to role)	First degree and PhD (or close to completion) in Chemistry, Materials Science, Physics, Chemical Engineering, or related field.	
Statutory, legal or special requirements		

Athena SWAN Silver Award

The University of Nottingham is focused on embedding equality, diversity and inclusion in all that we do. As part of this, we welcome a diverse population to join our work force and therefore encourage applicants from all communities, particularly those with protected characteristics under the Equality Act 2010.

Expectations and behaviours

The University has developed a clear set of core expectations and behaviours that our people should be demonstrating in their work, and as ambassadors of the University's strategy, vision and values. The following are essential to the role:

Valuing people	Is friendly, engaging and receptive, putting others at ease. Actively listens to others and goes out of way to ensure people feel valued, developed and supported.
Taking ownership	Is clear on what needs to be done encouraging others to take ownership. Takes action when required, being mindful of important aspects such as Health & Safety, Equality, Diversity & Inclusion, and other considerations.
Forward thinking	Drives the development, sharing and implementation of new ideas and improvements to support strategic objectives. Engages others in the improvement process.
Professional pride	Is professional in approach and style, setting an example to others; strives to demonstrate excellence through development of self, others and effective working practices.
Always inclusive	Builds effective working relationships, recognising and including the contribution of others; promotes inclusion and inclusive practices within own work area.

Key relationships with others