

## UNIVERSITY COLLEGE LONDON

### Research Associate – Coarse Graining of Stochastic Models of Heterogeneous Catalysts (PDRA)

#### Job Description

<b>Job Title:</b>	Research Associate – Coarse Graining of Stochastic Models of Heterogeneous Catalysts (PDRA)
<b>Department:</b>	Chemical Engineering
<b>Reports to:</b>	Dr Michail Stamatakis
<b>Grade:</b>	7
<b>Salary:</b>	£33,353 - £40,313 per annum inclusive of London allowance (depending on experience and qualifications)

#### Main Purpose

The aim of the project is to develop “Accurate and Computationally Efficient Models for Virtual Catalyst Design” and is funded by a Leverhulme Trust grant. The postholder will be required to carry out mathematical and computational research on the development of mesoscopic models of catalytic processes, by coarse-graining microscopic on-lattice kinetic Monte Carlo models. They will write up and present results at conferences and other professional meetings.

The post holder will collaborate with other members of Dr Stamatakis’ lab, as well as with researchers in the UK Catalysis Hub ([www.rc-harwell.ac.uk/UKCatalysisHub](http://www.rc-harwell.ac.uk/UKCatalysisHub)) and the Thomas Young Centre ([www.thomasyoungcentre.org](http://www.thomasyoungcentre.org)).

#### Duties and Responsibilities

- To develop and employ analytical and computational methods for coarse-graining microscopic models of reaction kinetics on heterogeneous catalysts (kinetic Monte Carlo-based models).
- To write reports, produce research publications, and present them at conferences and other professional meetings.
- Contribute to the preparation and drafting of research bids and proposals.
- Contribute to the induction, direction and management of undergraduate and postgraduate students, as requested.
- Collaborate with academic colleagues in the UK Catalysis Hub and the Thomas Young Centre.
- To contribute to the overall activities of the research group and Department, as required.
- This job description reflects the present requirements of the post, and as duties and responsibilities change/develop, the job description will be reviewed and be subject to amendment in consultation with the postholder.
- The postholder will carry out any other duties as are within the scope, spirit and purpose of the job as requested by the line manager or Head of Department/Division.

- The postholder will actively follow UCL policies including Equal Opportunities and Race Equality policies.
- The postholder will maintain an awareness and observation of Fire and Health & Safety Regulations.

Further details on Dr Stamatakis's research activities can be found at:

[www.homepages.ucl.ac.uk/~ucecmst](http://www.homepages.ucl.ac.uk/~ucecmst).

## UNIVERSITY COLLEGE LONDON

### Post-doctoral Research Associate – Coarse Graining of Stochastic Models of Heterogeneous Catalysts (PDRA)

#### Person Specification

##### Knowledge - including qualifications:

- Ph.D. in Theoretical Physics/Chemistry, Chemical Engineering, Applied Mathematics or related field.

##### Essential Skills:

- Demonstrated creativity and intellectual depth.
- Demonstrated research, and strong theoretical and computational skillsAbility to analyse and write up results and data.
- First authorship in high-impact journals.
- Ability to present complex information effectively to a range of audiences.
- Excellent written and verbal communication skills (memos, reports, publications, grants).

##### Essential Experience:

- Extensive experience in dynamic/kinetic Monte Carlo simulations for heterogeneous catalysis applications, statistical mechanics, and mean-field modelling.
- Extensive experience in computer programming in FORTRAN and/or C / C++.
- Experience of working in a research environment.
- Experience of multi-disciplinary working, including initiating research with a complementary technique.

##### Essential Personal Qualities:

- Commitment to high quality research.
- Ability to work collaboratively and as part of a team.
- Commitment to UCL's policy of equal opportunities and the ability to work harmoniously with colleagues and students from all cultures and backgrounds.