

PDRA in Computational Modelling of Heterogeneous Catalysis

We seek to appoint an innovative computational chemist with a broad range of experience in *ab initio* codes, data acquisition, and data analysis methodologies who will join the multidisciplinary MASI team. The Research Fellow will be appointed for two years and will bring expertise in computational modelling of heterogeneous catalysts, including interactions and bonding of small molecules (e.g. NH₃, H₂O, CO₂, H₂, N₂) with metal nanoclusters and chemical reactions on metals and hybrid interfaces.

The Research Fellow will be part of the Computational Materials Science group, led by Prof. Elena Besley (<https://ebesley.chem.nottingham.ac.uk/>).

The Research Fellow is expected to use high-performance computing to simulate interfacial chemical reactions and transport phenomena focusing on catalytic activity and selectivity of different metal nanoclusters in a range of chemical reactions. PhD in Chemistry, Physics, Chemical Engineering, or related field; knowledge of the concepts of density functional theory and first-principles molecular dynamics simulations; experience in the application of first-principles simulations to heterogeneous catalysis and complex reactive interfaces involving metal nanoclusters are essential.

This is a full-time (36.25h per week), fixed-term appointment of 2 years. Job share arrangements may be considered.

For informal enquiries contact Prof. Elena Besley, e-mail: elena.besley@nottingham.ac.uk.

Further details:

Our University has always been a supportive, inclusive, caring and positive community. We warmly welcome those of different cultures, ethnicities and beliefs – indeed this very diversity is vital to our success, it is fundamental to our values and enriches life on campus. We welcome applications from UK, Europe and from across the globe.

For all successful international applicants, including EU/EEA applicants from January 2021, we offer an interest-free loan to help cover the cost of immigration-related expenses to the UK, including visas and the NHS surcharge.