

PhD position at the University of Warwick (UK)

Title:

Quantum simulation of light-induced chemistry and electronic friction effects at metal surfaces

Project: A PhD studentship is available at the Department of Chemistry of the University of Warwick. The project will involve the quantum theoretical study of light-induced chemical reactions in industrially-relevant heterogeneous catalysis and gas-surface dynamics. Newly developed efficient ab-initio non-adiabatic dynamics simulation methods and high-performance supercomputing infrastructure will be used to study the role of light-matter interaction and molecule-surface energy transport in controlling chemical reactions at metal surfaces. The thereby gained understanding will guide the development of efficient light-assisted alternatives to industrial processes ranging from CO₂ capture to Carbon-Carbon coupling reactions. Depending on the student's interests, fundamental computational method development work can be a large part of this project.

How to Apply:

Please direct informal enquiries and requests for further information to Dr. Reinhard Maurer (r.maurer .at. warwick.ac.uk).

Please include your CV and a brief explanation of your interests in the research area of the studentship. Details on the formal application procedure can be found at <http://www.go.warwick.ac.uk/pgapply>