PhD Studentship

Dr Reinhard J. Maurer

**PhD project:** Quantum simulation of light-induced surface chemistry and electronic friction effects at metal surfaces

**Supervisor:** Dr. Reinhard J. Maurer

**Funding availability:** EU/UK (funded)

**Project description:**
A Ph.D studentship is available with a possible start date in Spring 2018. 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 quantum 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.

**Requirements:**
This studentship is open to UK or EU Nationals (fees paid, plus tax-free stipend - currently £14,553 per annum). Applicants should have an honours/Masters in chemistry. Prior experience in quantum chemistry and software development (e.g. Python) is desirable, but not essential. The successful candidate will be extensively trained in highly career-relevant molecular modelling and data analytics methods.

**How to apply:**
Please direct informal enquiries and requests for further information to Dr. Reinhard Maurer (r.maurer@warwick.ac.uk). Please include your CV and a brief explanation of your interests in the research area of the studentship. Research group information is available at warwick.ac.uk/maurergroup. Details on the formal application procedure can be found at http://www.go.warwick.ac.uk/pgapply.