Two PhD Studentships available

Dr. Reinhard J. Maurer & Dr. Scott Habershon

**PhD project:** Quantum dynamical simulation of tunnelling and electronic friction: what controls hydrogen chemistry on metals?

**Supervisors:** Dr. Reinhard J. Maurer and Dr. Scott Habershon

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

**Project description:**

Two computational chemistry PhD studentships are available with the earliest possible start date in September 2019.

Diffusion and reaction of atomic and molecular hydrogen at metal surfaces underpins a wide range of technological applications, including hydrogen dissociation in fuel cells, photoelectrochemical water splitting, hydrogen storage, and heterogeneous catalysis. The small mass of hydrogen means that quantum nuclear effects govern its chemical interaction with metal surfaces. In addition, electronic excitations in the metal can also affect the chemistry via so-called “electronic friction effects”. The two projects will involve the development and application of new quantum dynamical simulation methods based on path-integral molecular dynamics and nonadiabatic simulation methods to study the interplay between quantum tunneling and electronic friction in hydrogen metal chemistry.

The two projects will be closely aligned. Project 1 will involve the analytical method development and its application on hydrogen-metal diffusion. Project 2 will involve computational software development and its application to reactive hydrogen chemistry at metal surfaces.

**Requirements:**

These studentships are open to nationals of any country (fees paid, plus tax-free stipend - currently £14,844 per annum). The current funding covers tuition fees for EU and UK nationals. Applicants should have an honours/Masters in chemistry or physics. Prior experience in electronic structure theory, condensed matter theory, or software development (e.g. Python) is desirable, but not essential. The successful candidates will be trained in molecular modelling and data analytics methods.

**How to apply:**

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