

PhD Studentship in Modelling Molecule-surface Interactions and Solid/liquid Interfaces,
1788608

Applications from UK and EU citizens are invited for a 4-year PhD studentship in the group of Professor Alexander Shluger (UCL, UK, <http://www.alexshluger.com/>). This theoretical project will focus on modelling molecule-surface interactions and solid/liquid interfaces. Interfaces between solids and gases and solutions are ubiquitous in every-day environments. This project will investigate such interfaces at the nanoscale in strong collaboration with experimental studies using advanced TEM and Atomic Force Microscopy methods.

Studentship Description

Advanced TEM with the capability to image materials at 0.1 nm resolution even at gentle-beam conditions is ideally suited for atomic-scale studies of 2D materials. Recently, it has become possible to expose sample material to a gas while it is being observed in the STEM. The sample material can also be heated to a set temperature, and exposed to different gases. Such experiments will be used to study gas-solid interactions at the atomic scale. In contrast, AFM-based methods probe a small number of liquid molecules, typically located between a sharp tip and surface. Recent advances in liquid-environment AFM have enabled us to visualize three-dimensional (3D) hydration structures as well as two-dimensional (2D) surface structures with subnanometer scale resolution.

Theoretical models created in this project will be vital for understanding the results of such experiments. This will require developing new computational methods for quantum-mechanical and molecular dynamics simulations of 2D materials and insulators, their interaction with gas molecules, the effects of electron irradiation on the structure of materials, and reactions at surfaces, in relation to experiments. Atomistic simulations will be used to investigate resolution limits for imaging 3D distributions of ions and molecules at solid-liquid interfaces.

Person Specification

The successful applicant should have or expect to achieve at least a 2.1 honours or equivalent for undergraduate degree in Physics or Physical Chemistry. They will demonstrate strong interest and self-motivation in the subject, good experimental and computational skills, ability to think analytically and creatively. Good presentation and writing skills in English are required. Previous research experience in contributing to a collaborative interdisciplinary research environment is highly desirable but not necessary as training will be provided.

Eligibility

Please refer to the following website for eligibility criteria: <https://www.ucl.ac.uk/physics-astronomy/study/phd>

The start date is 23 September 2019. The studentship will cover all university fees and includes funds for maintenance at the standard UK rate and for participation in international conferences and workshops. This funding is for UK/EU nationals candidates.

Please submit applications in the following format:

A CV, including full details of all University course grades to date.

Contact details for two academic or professional referees (at least one academic).

A personal statement outlining what you hope to achieve from the PhD and your research experience to-date.

Please include a contact telephone number and an email address where you can be easily reached. References will be taken up for all short-listed candidates. Please contact Prof Alexander Shluger (a.shluger@ucl.ac.uk) for further details or to express an interest. Applications will be accepted until 30 March 2019 but the position will be filled as soon as an appropriate candidate is found.

Contact name

Alexander Shluger

a.shluger@ucl.ac.uk

<http://www.alexshluger.com/>