Two PhD Studentships in the Group of Prof. Alexander Shluger

Applications are invited for two PhD positions to work with Professor Alexander Shluger at the Department of Physics and Astronomy, University College London. The successful candidate will join a very active interdisciplinary group and will work on the theory and implementation of novel algorithms to model atomistic processes at interfaces of new functional materials using high performance computing.

The first project: Gas interactions with 2D materials at the atomic scale

This 3.5-year PhD studentship is available to the UK and EU students and is fully funded by the UCL-A*STAR Collaborative Programme via the Centre for Doctoral Training in Molecular Modelling and Materials Science (M3S CDT) at UCL. The student will be registered for a PhD at UCL where he/she will spend year 1 and the first six months of year 4. The second and third years of the PhD will be spent at the A*STAR IMRE in Singapore. The Studentship will cover tuition fees at UK/EU rate plus a maintenance stipend £17,050 (tax free) pro rata in years 1 and 4. During years 2 and 3, the student will receive a full stipend directly from A*STAR.

The Project

2D materials, such as graphene, MoS$_2$, hexagonal BN, black Phosphorus, are perspective materials for microelectronics, sensing, molecular membranes and other applications. Deep understanding of the interaction of surfaces of these materials with atoms and molecules is fundamental for success of these emerging technologies and requires developing new experimental and theoretical methods. This project combines experimental studies of these systems with theoretical modelling. It will use the most advanced aberration corrected scanning TEMs (STEMs) available at IMRE and computational modelling expertise and device manufacturing at UCL. Advanced microscopes with the capability to image materials at 0.1 nm resolution even at gentle-beam conditions are 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 all sorts of gas-solid interactions at the atomic scale. This includes gas-molecule adsorption, surface diffusion as well as catalysis and thin film growth.

The theoretical part of the project underpins these experiments and will be carried out both at UCL and at IMRE. It will involve quantum-mechanical and molecular dynamics simulations of 2D materials, their interaction with gas molecules, the effects of electron irradiation on the structure of materials, and reactions at surfaces in relation to experiments. The adventurous part of this program will involve linking the modelling of radiation effects induced by the electron beam of STEM with surface reactivity of 2D materials.
The second project: Molecular dynamics simulations of interface structure of Cu/TiW systems

The Studentship
This 4-year studentship is funded by EPSRC and Infineon Technologies AG and is open only to UK applicants and EU applicants resident in the UK for the last three years. The PhD training and research will be carried out within the M3S Engineering Doctorate Centre at UCL and the London Thomas Young Centre https://www.thomasyoungcentre.org/ in collaboration with Materials Center Leoben, Austria https://www.mcl.at/.

The Project
Understanding of adhesion between metal layers is fundamental to any nano-electronic device. For example, signal delay and the electromigration failure at interconnects are important problems for fabricating reliable future devices. This project will therefore focus on modelling atomistic processes at Cu/TiW interfaces used in many devices. It will involve testing and developing force-fields or semi-empirical interatomic potentials for Cu, TiW, and Cu/TiW interface and for the interaction of O and H2O with these systems. This should allow us to make calculations for large (tens of thousands of atoms) interface models and to simulate complex morphologies, including dislocations and grain boundaries. We will run molecular dynamics simulations for Cu/TiW interfaces at realistic temperatures, such as 400 C, for realistic times, such as tens of nanoseconds. This will provide understanding of thermomechanical fatigue experiments at Infineon and the role of oxygen and water in embrittlement and delamination of these systems.

The Candidate
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 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.

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 2018 but the position will be filled as soon as an appropriate candidate is found.