

Molecular Dynamics Simulations of Graphene-Protein interactions for Biomedical Diagnostic Sensors

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Applications are invited for a three-year MPhil/PhD studentship. The studentship will start on **1st October 2020**.

Project Description

Fundamental understanding of protein dynamics, energy landscape and conformational changes, is central to deeper insights into a protein's specific biochemical functions (such as allosteric signalling, enzyme catalysis etc.). This could aid in drug discovery, novel protein engineering and distinguishing between normal and pathogenic conformational changes for disease diagnostics applications. In this project we aim to investigate a novel approach for the detection of protein dynamics and interactions on the surface of Graphene (and related two-dimensional materials, G2DM) through direct comparison of Molecular Dynamics Simulations (MDS) with experimental results obtained from our G2DM based sensors developed at the University of Plymouth in collaboration with the University of Cambridge.

For the MDS we will employ the Kohn–Sham (KS) formalism of the density functional theory approach to perform the in-silicio study of the graphene-protein system. The KS approach has proven to be one of the most efficient and reliable first-principles methods for investigating material properties and processes that exhibit quantum mechanical behaviour. The pioneering nature of this research will enable the student to use BigDFT massively parallel electronic structure code to simulate the graphene-protein sensor, based on the High Performance Computing Cluster at the University of Plymouth, as well as making comparisons with cutting-edge experimental measurements. Accurate comparisons between MDS and experimental results has the potential to lead to a breakthrough in our understanding of protein dynamics and conformational states, thus opening a plethora of applications in diagnostics, prognostics and therapeutics particularly for Alzheimer's, cancer and cardiovascular diseases.

Eligibility

Applicants should have (at least) a first or upper second class honours degree in an appropriate subject and preferably a relevant MSc or MRes qualification. Some experience of quantum mechanics or solid-state physics and scientific programming using a language such as python, C or Fortran is desirable.

The studentship is supported for 3 years and includes full Home/EU tuition fees plus a stipend of £13,863 per annum. The studentship will only fully fund those applicants who are eligible for Home/EU fees with relevant qualifications. Applicants normally required to cover overseas fees will have to cover the difference between the Home/EU and the overseas tuition fee rates (approximately £9,950 per annum).

If you wish to discuss this project further informally, please contact Dr Shakil Awan (shakil.awan@plymouth.ac.uk) or Dr Vincent Drach (Vincent.drach@plymouth.ac.uk). However, applications must be made in accordance with the details shown below.

For an application form and full details on how to apply, please visit www.plymouth.ac.uk/postgraduate. Applicants should send a completed application form along with a covering letter detailing their suitability for the studentship, C.V., and 2 references to Graduate School, Link Building, Level 3, Plymouth PL4 8AA or e-mail scienvresearch@plymouth.ac.uk.

The closing date for applications is 12 noon on 17th April 2020. Shortlisted candidates will be invited for interview week commencing 4th May 2020. We regret that we may not be able to respond to all applications. Applicants who have not received an offer of a place by 15th May should consider their application has been unsuccessful on this occasion.