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PhD studentship “First principles molecular dynamics simulation of
electron transfer across solid/liquid interfaces” – University College London (UK)

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A PhD studentship is available to work under the supervision of Professor Jochen Blumberger at the Condensed Matter and Materials Physics Laboratory, University College London, UK. The project involves the development and application of first principles molecular dynamics methods for the simulation of electron transfer across solid/liquid interfaces. Such reactions are at the heart of pressing societal and environmental issues such as artificial photosynthesis and solar fuel production, decontamination of soil and geochemical transformations. In the project we will adopt and further develop a dedicated density functional theory-based method to compute the parameters governing electron transfer reactions between redox active solvated species and semiconducting electrode materials. This will give us access to a detailed atomistic understanding of the thermodynamics, kinetics and mechanism of interfacial redox processes underpinning the rational design of improved electrode materials for energy applications and the geochemical cycling of metal ions. Access to high performance computing facilities will be provided. Interested candidates may want to take a look at recent group publications in the field, listed on the group website <http://www.blumberger.net>.

Highly motivated students from Physics, Chemistry or Materials Science Departments are strongly encouraged to apply for this post. Due to funding restrictions only UK or EU citizens are eligible to apply. The candidate should have, or be about to receive, an honours degree (at least II.1 or equivalent) in Physics, Chemistry or a related subject. Good knowledge in quantum mechanics and statistical mechanics is expected and interest in writing computer code and shell scripts is an advantage. Some experience with molecular simulation is desirable, but not essential. The studentship will cover all university fees and includes funds for maintenance at the standard EPSRC rate. The studentship will start 1. October 2018.

Applications should include (i) a motivation statement (250 words max) briefly describing any previous research projects you worked on and why you would like to apply for this post (ii) a CV (2 pages max) including publications (if any) (iii) transcripts of undergraduate (Bachelor) and graduate (Master) studies (iv) names, contact details and email addresses of 2 referees. Please send these four application documents as a single zip file to Jochen Blumberger, j.blumberger@ucl.ac.uk specifying in the subject line “PhD application”. Candidates are advised to apply as early as possible as the selection process will commence immediately and continue until a suitable applicant is found. All applications received until 31. December 2017 will be considered.

Informal enquiries regarding the vacancy can be made to Jochen Blumberger, j.blumberger@ucl.ac.uk. For any administrative queries regarding the application process, please contact James Gane, james.gane@ucl.ac.uk.