Post-doctoral Research Assistant in Computational Physics/Chemistry, University College London (United Kingdom)
Department of Physics and Astronomy

Two postdoctoral research positions are available in the research group of Professor Jochen Blumberger at University College London, Department of Physics and Astronomy. The positions are funded by the ERC grant “SOFTCHARGE: Charge carrier transport in Soft Matter: From Fundamentals to High Performance Materials”, which aims at a fundamental understanding of the nature and transport mechanism of charge and excitation energy carriers in organic materials using novel non-adiabatic molecular simulation approaches. In the project you will add new functionalities to our recently developed non-adiabatic molecular dynamics code (J Chem Phys 145, 64102, 2016) and/or investigate structure-function relationships in organic materials. Work may be carried out on one or several of the following topics:

(i) development of non-adiabatic molecular dynamics frameworks beyond surface hopping including incorporation of nuclear quantum effects (ii) extension of current implementation to enable simulation of exciton transport and dissociation (iii) machine learning of excited state energies and gradients (iv) prediction/building of structural models for crystalline and amorphous organic materials (v) establishing structure-charge mobility relationships for 2D and 3D organic materials (crystals, thin films, organic interfaces).

Access to high performance computing facilities will be provided.

The positions can be taken up from 1 February 2018, the start date should be no later than 1. October 2018. This project is funded by ERC for 1 year in the first instance, with the option to extend for another 2 years (3 years in total).

Eligible candidates have a PhD in computational physics/chemistry or related disciplines. Highly motivated individuals who have a strong background in computer code development (fortran, C++ or similar) or in the structure prediction and modelling of organic materials are especially encouraged to apply for this post. Strong interest in the simulation of charge/excitation energy transport phenomena in organic and biological materials is essential. Good knowledge in molecular quantum mechanics, statistical mechanics and molecular simulation methods is expected. First-hand experience with advanced molecular dynamics simulation techniques (e.g. Ehrenfest, surface hopping, exact factorization or path integrals) is an advantage but not required.

Applicants should apply online at
https://atsv7.wcn.co.uk/search_engine/jobs.cgi?SID=amNvZGU9MTY5NDAzNyZ2dF90ZW1wbGF0ZT05NjUmb3duZXI9NTA0MTE3OCZvd25lcnR5cGU9ZmFpciZicmFuZF9pZD0wJnBvc3RpbmdfY29kZT0yMjQ=
Ref No 1694037.Online application involves upload of (i) Statement in support of your application (ii) CV (iii) full list of publications as supporting document and (iv) contact details of 2 referees. The closing date for applications is 31. December 2017.

Interested candidates may want to take a look at recent group publications in the field, listed on the group website http://www.blumberger.net Informal enquiries regarding the vacancy can be made to Professor Jochen Blumberger by email, j.blumberger@ucl.ac.uk. If you have any administrative queries regarding the application process, please contact James Gane, james.gane@ucl.ac.uk (Tel +44 (0)20 7679 7143).