RESEARCH ASSISTANT

Job/Fellowship Reference: CONT_DOUT7120/ICETA/75006/10989/12/2008
Main research field: Chemistry
Sub research field: Computational Chemistry/Chemical Physics

Job summary:
Modeling of Ionic Liquids

ICETA (Instituto de Ciências e Tecnologias Agrárias e Agro-Alimentares) invites applications for a Researcher position (equivalent to "Investigador Auxiliar" in the Portuguese "Estatuto de Carreira de Investigação") to work at the University of Porto (Portugal), in the area: *modelling of ionic liquids*.

Job/Fellowship description
Modelling of ionic liquids

Ionic systems with low melting temperature, previously called as room temperature molten salts, are now simply called ionic liquids (*ILs*). In the last decade, ILs have emerged as promising solvents for environmentally friendly organic synthesis, electrodeposition, and electrolytes for electrochemical devices. In fact, the most common application of ILs is their use as alternative solvents in industrial applications. Despite this technological interest, a detailed microscopic view of the role played by the structure and the dynamics of ILs as reaction media is still lacking.

Computer simulation has become a well-used method for studying ionic liquids. Current state-of-the-art includes work right across the time and length scales encompassing for instance, anisotropic single site potentials, multi-site coarse-grained models and atomistic modelling. The first generation of challenges has been met, and it is now possible to make predictions for key materials properties of ILs and even to investigate a chemical reaction therein. Our group (Material Chemistry Group of ICETA/ Centre of Chemistry of the University of Porto – CEQUP/REQUIMTE) aims to address this issue by

performing a theoretical study for revealing the microscopic structure, thermodynamics, and dynamics of pure ILs and interfaces of ILs with non-ILs.

ICETA (Instituto de Ciências e Tecnologias Agrárias e Agro-Alimentares) invites applications for a research position in the area of Modelling of Ionic Liquids, to work at the University of Porto (Portugal) at the Materials Chemistry group (www.fc.up.pt/pessoas/ncordeir/).

Personal Profile:

The candidate should hold a Ph.D. in Chemistry, Physics, Material Sciences, Chemical Engineering or a related subject. Further, he/she should be a routine user of classical Molecular Dynamics/Monte Carlo and preferably be familiar with *ab initio* simulations. Some knowledge of ionic liquids will be appreciated.

Applicants should have 3 years experience at post-doc level (Justified exceptions can be accepted, in accordance to FCT regulations), and a good publication record.

It is expected that the future research assistant will publish his work in good journals of this area. We would like the future Research Assistant to develop his/her own research in within the activities of the host laboratory. The candidate should also supervise students, as well as participate in on-going research projects of the host and some managerial jobs of the computing lab. We hope that the candidate will develop and manage new projects.

Support will be provided, including access to joint research and laboratory equipment. We are committed to foster gender-equality in Science.

Call Deadline – 15th October 2012.

Gross salary – 3,191.82€/month (including health insurance)

Applications should include CV, the names and contact details of two referees, copies of the certificates of academic degrees and passport/identity card, and should be submitted by e-mail to ncordeir@fc.up.pt.