LINKÖPING UNIVERSITY

26 december 2016

Postdoctoral Researcher in *ab initio* and/or Molecular Dynamics simulations of conducting polymers

A postdoctoral research position is available at the Laboratory of Organic Electronics, Linköping University (Campus Norrköping), Sweden starting winter/spring 2017. The Laboratory of Organic Electronics is renowned for its world-leading research on electronic devices based on organic electroactive materials. Its primary theme involves the coupling of ions and electrons as signal carriers for applications in organic bioelectronics, printed electronics, organic solid-state and electrochemical devices. Currently, the research staff of the Laboratory includes about 50 researcher (professors, senior and junior scientists and PhD students), see http://fe.itn.liu.se/orgel for detail.

Background and duties: Among all organic materials conducting polymers have become the material of choice for many electronic and bioelectronics devices including OLED, photovoltaic cells, ionic and electrochemical transistors, sensors, neural probes and many others. Another area where conductive polymers can be highly competitive is a large-scale energy storage and power electronics utilizing mixed electronic-ionic conductors in devices such as supercapacitors, batteries and fuel cells.

An experimental progress and development of the above devices is difficult without fundamental understanding of the basic material properties. The main aim of the research project is to perform computational studies of conducting polymers (in particular, PEDOT) using *ab initio* and/or Molecular Dynamics simulations to answer fundamental questions concerning morphology, polymerization, ion diffusion, role of water and solvents; mechanisms, pathways and kinetics of oxidation and reduction reactions in these materials, and many others. The theoretical work will be performed in a multidisciplinary environment with strong interaction with experimental groups in the Laboratory, where the obtained theoretical results will help to understand and guide the material engineering and device design for better and enhanced performance.

Qualifications: The applicant must have, or be about to receive a doctoral degree in a subject relevant to the research project (e.g. physics, applied physics, chemistry, theoretical chemistry, biophysics, etc.) and needs to be passionate about research. Problem solving ability and creativity, as well as the ability to work independently are essential. Another prerequisite is knowledge and good skills in programming. Experience with *ab initio* and/or Molecular Dynamics simulations is desirable.

Appointment: initially for one year with a possibility of an extension for the second year depending on a mutual agreement and performance. Starting time is winter/spring 2017. The fellowship amounts to SEK25000:-/month (tax-free) (~€2500/month).

Application procedure: The application should be sent electronically to Prof. Igor Zozoulenko (igor.zozoulenko@liu.se) with a subject line "postdoc computational studies of conducting polymers". The application should include a cover letter, a CV (with names of two references), a publication list, and other documents you may wish to refer to. (All abovementioned documents should be sent as a single pdf-file). In addition, maximum of three selected publications can be enclosed with the application. Screening of candidates will start in January 2017 and will continue until the position is filled.