UNIVERSIDADE DE SÃO PAULO
INSTITUTO DE FÍSICA

PhD position: X-ray nano-tomography of photoactive polymers

Today, polymers are the focus of many research groups throughout the world, encompassing a variety of fields such as Energy Conversion and Neuroscience. In photovoltaic applications, organic solar cells based on polymers take advantage of bulk hetero junction architecture to maximize the probability of charge pair separation and limit the charge recombination process. In Neuroscience, polymers are investigated as a bio-compatible material that acts as photo-activated charge donor capable of restoring light sensitivity in degenerated retinas [1].

In parallel with the developments in Materials Science, recent advances in X-ray instrumentation (sources and optics) are opening fantastic opportunities to look at materials in a way that has never been possible before. The highly penetrating power of X-rays make them ideal for probing the dynamic structure of realistic, functioning devices for energy conversion and storage, but this is an application that is largely unexplored. With the advances in imaging techniques where combination of better optics for hard X-ray focusing, new measuring schemes, and algorithms taking advantage of coherent X-ray illumination, the potential for sub-nm resolution is within reach.

Because of the hard X-ray penetration, complementary analysis techniques and non-ambient sample environments are relatively easy to integrate with the X-ray experiment for *in situ* studies. These methods will be applied to real devices for resolving problems relating to up-scaled processing of nano-structured devices, among which polymer solar cells. The *in situ* experiments will be applied to advance the fundamental understanding of the formation of polymer solar cell nanostructure and its development and stability with respect to thermal and solvent annealing, and with light soaking.

In this project, the PhD candidate will investigate the nanostructure of polymer-electrolyte interfaces under several conditions and, in collaboration with research groups at Denmark, will work on improving algorithms for 3D reconstruction of phase contrast X-ray projections, typically from ptychographic tomography (ptychography is a form of phase contrast imaging, exploiting coherent X-ray illumination). 3D resolution depends on X-ray beam and sample positioning stability, and not least, on the algorithms for aligning projections and reconstructing the phase tomogram. The standard way of reconstructing tomograms from 2D ptychography projections is the well established filtered back projection, reconstructing the tomogram slice by slice, but much more advanced algorithms for 3D reconstructions have been developed, and research is still in advance in this direction. The knowledge acquired in this collaborative project will be useful at the nanobeam line of the new Brazilian synchrotron, as well as in protein crystallography with free electron lasers.

[1] Ghezzi *et al.* Nature Photonics **7**, 400–406 (2013)

Qualifications and specific competences: Applicants with MSc degree in physics or nanotechnology and good skills in mathematics and programming (matlab, python, C) are preferred.

Place of Employment and Place of Work: Department of Applied Physics, University of Sao Paulo, Sao Paulo, Brazil. Department of Energy Conversion and Storage, Technical University of Denmark, Risø Campus, Frederiksborgvej 399, DK-4000 Roskilde.

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