Internship proposal starting ASAP

(Posted Jan. 24, 2014)

Topic: Multiscale modeling and numerical simulation of degradation layer growth in dye-sensitized solar cells.

Advisors: Prof. A.A. Franco in collaboration with Dr. Fréderic Sauvage from Laboratoire de Réactivité et de Chimie des Solides (LRCS) and with Prof. Jean-Paul Chehab and Dr. Youcef Mammeri from the Laboratoire Amiénois de Mathématiques Fondamentales et Appliquées (LAMFA) - 33 rue St. Leu, 80039 Amiens Cedex, France.

Context and objectives: Dye-sensitized solar cells is a photovoltaic alternative to silicon developed worldwide as it gathers a set of advantages such as low-cost and easy production, high power conversion performances under shadowed sky and diffuse light, low sensitiveness to temperature fluctuations, can be flexible and bifacial etc… However, the main constrain of this technology for its successful market integration in niche is its lack of stability at temperatures greater than 60°C[1].
Recently, LRCS has pointed out the formation of a chemical degradation layer forming at this temperature and beyond which has a strong outcome for the cell operation while giving answer to long-term numerous speculations raised in the literature. Although such area is dominated by chemists and physicists, a mathematician will be integrated in this research project for which this internship will call for multi-scale modeling and numerical simulation of first the conformal growth of this degradation layer within a randomly distributed monomodal mesoporous electrode. This model will be developed using Matlab environment and within the LRCS computational framework MS LIBER-T[2],[3] to describe the transport of ions and subsequent electrochemical reactions within porous electrode. Sensitivity analysis of the model to different microstructural parameters will be carried out. This model will be used to provide interpretation of experimental data and to guide experimentalists in how to reconsider the existing configuration.

Necessary skills: applied mathematics, numerical methods, physics (equivalent to French Master 1 or Master 2).

Contact:

Prof. Alejandro A. Franco
Laboratoire de Réactivité et de Chimie des Solides (LRCS), UMR CNRS #7314
Université de Picardie Jules Verne
33, rue Saint Leu - 80039 Amiens, FRANCE
Phone: 0033 3 22 82 75 86

E-mail: alejandro.franco@u-picardie.fr
LRCS homepage: http://www.u-picardie.fr/labo/lrcs/
RS2E homepage: http://www.energie-rs2e.com/fr
Research & teaching homepage: www.modeling-electrochemistry.com

[1] M. Flasque, A. Nguyen Van Nhien, J. Swiatowska, A. Seyeux, C. Davoisne, F. Sauvage, *ChemPhysChem* (2014) in press, http://dx.doi.org/10.1002/cphc.201300904
[2] A.A. Franco, *RSC Advances*, **3** (32) (2013) 13027.
[3] www.modeling-electrochemistry.com