European Research Council

ERC Advanced Grant 2011
Research proposal (Part B1)[1]

Understanding Ion Transport in Nanoporous Carbons; application to Energy Storage and Sustainable Development

IONACES

Cover Page:

- Name of the Principal Investigator (PI): Patrice SIMON
- Name of the PI's host institution for the project: Université Paul Sabatier – Toulouse III
- Proposal full title:
  Understanding ion transport in nanoporous carbons: application to energy storage and Sustanable development
- Proposal duration in months 60 months

Proposal summary (half page)
Electrochemical Double-Layer Capacitors Electrochemical Capacitors (EDLC) are promising devices for clean energy storage applications. In EDLCs, the charges are stored electrostatically at the electrolyte / electrode interface, which confers them high power and cycling capabilities. Until recently, it was believed that charge storage in porous carbon EDLC electrodes could be achieved only if the pore size of the carbon was larger than the electrolyte ions with their solvation shells. Using Carbides Derived Carbons (CDCs) which have controlled pore sizes between 0.6 nm and 1.1 nm, we recently demonstrated that high capacitive performances could be obtained when the pore size is smaller than the solvated ion size. The origin of this capacitance increase is still unclear despite important modelling efforts achieved by many research groups.
Using our fine-tuned, controlled pore size CDCs carbons with narrow pore size distribution, we propose here an integrated approach combining the use of experimental electrochemical methods (EQCM, EIS, CV…) and in-situ analytical techniques (NMR, XRD), to computational modelling (Molecular Dynamics, Monte Carlo and Reverse Monte Carlo methods) to elucidate the ion transport and adsorption mechanisms in confined nanopores.
A direct application of this fundamental approach concerns the energy storage with supercapacitors. Thanks to the unique features offered by the CDCs, we propose to develop the next generation of high-energy density micro-supercapacitors from bulk CDC films.
The evidence of the increase of the capacitive ion adsorption associated with ion partial desolvation in micropores is also of great interest in different areas such as water desalination. CDCs, which have demonstrated volumetric capacitance improvement of 100% compared to activated carbon for supercapacitor application, are appealing materials for water desalination applications, which will be the last part of the project.

[1] Instructions for completing Part B1 can be found in the Guide for Applicants for the Advanced Grant 2011 Call

Section 1: ***The Principal Investigator (see Guide for Applicants for the Advanced Grant 2011 Call – Instructions for completing "Part B" of the proposal)***

1(a) Scientific Leadership Profile (max 1 page)

My work is focused onto the modification of interfaces at electrodes for electrochemical energy storage applications, and more specifically for Electrochemical Double Layer Capacitors (supercapacitors).

Unlike traditional batteries, supercapacitors store electricity electrostatically by physically separating positive and negative charges along two electrical conductors: electrolyte ions and highly porous carbon electrodes.

In 2006, we have shown that, ***defying conventional wisdom, powerful supercapacitor electrodes could be developed by designing porous carbons with pores smaller than the size of solvated ions***. Using tunable, controlled and narrow pore size distribution carbons as model materials, namely carbide-derived carbon (CDC), we found that ***carbon with 0.7-0.8 nanometer pores could increase the amount of volumetric electrical charge by 100%***, an effect we assigned to the ***deformation of the solvation shell of solvent molecules surrounding the ion***. This paper received an important interest from the scientific community (see section 1.c Science 2006 cited 345 times). Using solvent-free electrolytes, we then demonstrated that a ***maximum of capacitance was observed when the carbon pore size was in the same range of the ion size*** (Nature Materials 2008 cited 495 times, JACS 2008, cited 120 times). Also surprisingly is that the kinetics of the ion migration insides these sub-nanometer pores is still high, thus maintaining high power for the EDLC electrodes (Electrochimica Acta, 2010). These findings highlight the lack of fundamental understanding of the electrochemical behaviour of ions confined in nanopores. They also rule out the conventional conception of the double layer, with solvated ions adsorbed on each side of the carbon pore wall consistent with the absence of a diffuse layer in sub-nanometre pores.

These results conferred to our group a leading position in the research on supercapacitors. They opened new research directions directed towards the basic understanding of the ion transport in nanopores, as well as the charge storage mechanism in this confined environment. As a result, several groups achieved modelling work and confirmed our results (Kornyshev's group, Imperial College, UK; Meunier's group, Oak Ridge Lab, US; Kaneko', Shinshu University, Japan; Kim', Carnegie Mellon Univ., US; Borodin' from Utah Univ., US (…) but the charge storage mechanism and the ion environment are still unclear.

I have been asked to write several invited papers on carbons for supercapacitors for different journals such as Science (2008, see paper #6 section c), Fuel Cells (2010), Philosophical Transaction of the Royal Society (2010), Journal of Materials Research (2010), The Electrochemical Society Interface (2008), Accounts of Chemical Research (in progress)..

I tried to inspire young researcher by transmitting my passion for research. Christel Portet (PhD in 2006) who received the "Délégation Générale pour l'Armement National PhD prize 2005", is now employed at the CEA (Grenoble, France). Julie Segalini, currently PhD student in the group, received the Best Poster Award at the International ISEECAP Metting in 2009. C. Largeot (PhD in 2009) is employed at the Leitat technological Center in Barcelona (Spain). M. Chakir (Post Doc 2009) has been hired by the Renault Company. L. Bazin (PhD 2010) is now Engineer in the Microconnections Company in Mantes-la-Jolie (France); Pierre-Louis Taberna (PhD 2002) is now CNRS Researcher in my group. S. Mitra (Post Doc 2007) and M. Manikoth (Post Doc 2010) are now Associate Professor at the Bombay Institute of Technology and at the Thiruvananthapuram Institute of Science. E. Perre (PhD 2010) is Post Doc at UCLA (US). As of today, all my former PhD students and Post Doc found a position.

One part of my neighbouring research activities not directly concerned by the present proposal is directed towards the Li-ion batteries and more specifically to the nano-structuration of the electrode / electrolyte interface. This part of my activity is developed in the frame of the ALISTORE European Research Institute, with gathers European 21 laboratories and 15 companies in Europe (see http://www.alistore.eu/). ALISTORE-ERI has been created by Prof. Jean-Marie Tarascon (Amiens University) to federate the European research onto Advanced Li-ion batteries. Since July 1st 2010, I have been elected as Director of the ALISTORE-ERI, which is a Research Federation CNRS n°3104.

Last but not least, the French Ministry of Research together with the CNRS announced in July 2010 the creation of the French network on Electrochemical Energy Storage (RS2E) with the objective to build a coherent French scientific landscape in the field of energy storage. Prof. J.M. Tarascon (as Director) and I (as associate director) are in charge of this network that will start in May 2011. Additionally, I will ensure the scientific leadership and coordination of the Supercapacitor research thematic