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

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GENERAL CONTEXT AND GOALS

In the past decade, lot of attention has been put on electrochemical double layer capacitors (EDLCs), also known as supercapacitors, for high power delivery or energy harvesting applications. The charge storage mechanism in supercapacitor electrodes relies on electrostatic attraction between the electrolyte ions and the charges at the electrode surface, leading to a charge separation at the electrolyte/electrode interface. In 2006, the discovery of the capacitance increase in carbon nanopores opened new opportunities for these systems. However, the origin of this capacitance increase was still. This highlighted the need for 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 inside nanopores, which was the target of this project. The project is based on the use of our fine-tuned, narrow pore size distribution CDCs carbons, and CDCs synthesis and structural characterizations will be done as the first task. CDCs have been used as well for preparing micro-supercapacitor devices as well as for water desalination applications which will be the last part of the work

KEY RESULTS

- First modelling of ion adsorption using realistic carbon nanostructures (Nature Materials 2012)

- Molecular Dynamics modelling studies showed partial ion desolvation in carbon nanoppores in neat ionicl liquid electrolyte

- In presence of solvent molecules, Molecular Dynamics modelling studies confirmed ion desolvation in carbon nanopores
- Evidencing ion exchange mechanisms in carbon nanopores thanks to the use of in-situ Electrochemical Quartz Microbalance tool (JACS 2014)

- Combined in-situ NMR and EQCM with in-EQCM to show different ion storage mechanisms in carbon nanopores vs the electrode polarity (Nature Mat, 2015)

- Concept of pseudocapacitive Li-ion inercalation reaction in organic electrolytes thanks to the use of nano-sized Nb2O5 particles (Nature Materials 2013)

- Evidence of multi-valent ion intercalation in new 2-Dimmensional Mxene materials (Science 2013)

- Design of the first on-chip micro-supercapacitor using Cabide Derived carbon films (Science 2016)

SCIENTIFIC PRODUCTION

29 papers, including Science (7) and Nature Publishing Group (4)

7. "Efficient storage mechanisms for building better supercapacitors"
M. Salanne, B. Rotenberg, K. Naoi, K. Kaneko, P.-L. Taberna, C.P. Grey, B. Dunn, P. Simon, ***Nature Energy*** 1, 16070 (2016),
6. "On-chip and free-standing elastic carbon films for micro-supercapacitors"
P. Huang, C. Lethien, S. Pinaud, K. Brousse, R. Laloo, V. Turq, M. Respaud, A. Demortière, B. Daffos, P.L. Taberna, B. Chaudret, Y. Gogotsi and P. Simon, ***Science*** 351, 6274 (2016) 691-695
5. "In situ NMR and electrochemical quartz crystal microbalance techniques reveal the structure of the electrical double layer in supercapacitors"
J. M. Griffin, A. C. Forse,W.-Y. Tsai, P.-L. Taberna, P. Simon C P. Grey, ***Nature Materials*** (2015)
4. "Where do batteries end and supercapacitor begin?"
P. Simon, Y. Gogotsi and B. Dunn ***Science*** 343, 1210 (2014).
3. "Cation intercalation and high volumetric capacitance of two-dimensional titanium carbide."
M. M. Lukatskaya, O. Mashtalir, C. Ren, E. Chang, Y. Dall'agnese, P. Rozier, P.L. Taberna, M. Naguib, P. Simon, M. Barsoum, Y. Gogotsi, ***Science*** 341 (2013) 1502-1505.
2. "Evidence of intercalation pseudocapacitance in high-rate lithium-ion energy storage materials",
V. Augustyn, J. Come, M. A. Low, J. W. Kim, P.-. Taberna, S. H. Tolbert, H. D. Abruña, P. Simon, and B. Dunn, ***Nature Materials*** 6 (2013) 518-522.
1. "On the molecular origin of supercapacitance in nanoporous carbon electrodes"
C. Merlet, B. Rotenberg, P.A. Madden, P.-L.Taberna, P. Simon, Y. Gogotsi, and M. Salanne, ***Nature Materials*** 11 (2012) 306-310.

KEY NUMBERS

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