MERLET Céline merlet@chimie.ups-tlse.fr
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CNRS researcher

CIRIMAT – Université Paul Sabatier
https://sites.google.com/view/celinemerlet/home

RESEARCH EXPERIENCE

July 2017 – Present

CNRS researcher at the CIRIMAT laboratory (www.cirimat.cnrs.fr), developing multi-scale models for the study of electrochemical energy storage systems. Work done in collaboration with the RS2E network (www.energie-rs2e.com/en).

October 2013 – June 2017

Post-doctoral researcher in the Department of Chemistry at the University of Cambridge (www.ch.cam.ac.uk), developing a new simulation method to examine the complex electrode/ electrolyte interface in supercapacitors in strong association with *in situ* NMR experiments. Working in the group of Pr. Clare Grey (www-grey.ch.cam.ac.uk) in collaboration with the group of Pr. Daan Frenkel (www-frenkel.ch.cam.ac.uk).

October 2010 – September 2013

PhD in the PECSA laboratory (Physicochimie des Electrolytes, Colloïdes et Sciences Analytiques, www.pecsa.upmc.fr) working on realistic models of ion adsorption in carbon micropores through state of the art molecular dynamics simulations, supervisor: Dr. M. Salanne; head of the laboratory: Pr. P. Levitz.

Academic visits during the PhD:

CIRIMAT laboratory, Université Paul Sabatier, Toulouse: experimental electrochemical caracterisations of carbon/carbon supercapacitors.

Susan Perkin's group, University of Oxford : discussions about the utilisation of a surface force apparatus for the study of the mica/ionic liquid interface.

February 2010 – August 2010

Six-month research internship in the MML at the University of Oxford (Materials Modelling Laboratory, http://mml.materials.ox.ac.uk), working on molecular dynamics of molten fluorides on the one hand, and molten silicates on the other hand; supervisor: Pr. P. Madden; head of the laboratory: Pr. N. Marzari.

March 2009 - August 2009

Six-month research internship in the Structural Bioinformatics laboratory in the Pasteur Institute (http://www.pasteur.fr/recherche/unites/Binfs). Working on the dynamics of a histidine kinase (DesK) using classic and targeted molecular dynamics; supervisor and head of the laboratory: Dr. M. Nilges.

November 2008

Research internship in the LI2C laboratory (laboratoire des Liquides Ioniques et Interfaces Chargées) at UPMC (http://www.pecsa.upmc.fr/), working on molecular simulation of the molten salts LiF and KF. Learning about the theory of molecular dynamics and about the software used in simulation; supervisor: Dr. M. Salanne; head of the laboratory: Pr.V. Cabuil

EDUCATION

September 2013

- PhD, Physical Chemistry, Université Pierre et Marie Curie (Paris)
  Modélisation de l'adsorption des ions dans les carbones nanoporeux
  (Modeling ion adsorption in carbon nanopores)

September 2010

- Master of Science degree of chemistry, Université Pierre et Marie Curie
- French "diplôme d'ingénieur Chimie ParisTech"

July 2008

- Bachelor of Science degree in chemistry and engineering at Chimie ParisTech

AUTHORING ACTIVITIES

Publications Author of **31 publications**
Author of **2 book chapters**
(A complete list of my publications is provided at the end of this document.)

Conferences Author of **49 talks** and **7 posters** given in national or international conferences, including **16 invited talks** in international conferences
(A complete list of my presentations is provided at the end of this document.)

TEACHING EXPERIENCE AND SUPERVISION

PhD
- Anagha Sasikumar, since october 2019, as PhD director, co-director: Pr. P. Simon
- El Hassane Lahrar, since october 2017, as co-director, PhD director: Pr. P. Simon
- Amangeldi Torayev, 2016-2019, co-supervisor, co-directors: Pr. C. Grey at the University of Cambridge and Pr. A. Franco at Université Picardie Jules Verne

Master
- Amangeldi Torayev, 2015, student of the MESC Master (Materials for Energy Storage and Conversion)

Post-doc
- El Mahdi Halim, since 2020, co-supervised with P.-L. Taberna and P. Simon
- Dimitrios Kilymis, 2018-2020, in collaboration with C. Pickard and A. Bartók
- Anouar Belhboub, 2017-2019

2019 Graduate courses on Molecular Dynamics Simulations

2014 Senior demonstrator in the practical component of the inorganic chemistry class in the Department of Chemistry at the University of Cambridge (8h)

2010 - 2013 Teaching assistant in chemical kinetics and thermodynamics of 2nd year of higher education pupils at Université Pierre et Marie Curie (64h/year)

2008 - 2009 Oral examiner in chemistry of 2nd year of higher education pupils (2h/week)

ORGANISATIONAL ROLES

2019-2020 Co-organisation of JTMS ("Journées Théorie, Modélisation et Simulation")

Since 2019 Board member of subdivision "Modélisation et Simulation" of the "Division Chimie Physique" of the "Société Chimique de France"

August 2017 Co-organisation of the symposium "In situ / operando and computational studies of electrochemical energy materials" at "International Materials Research Congress 2017" conference

May 2017 Co-organisation of the Grey group retreat

2016 - 2017 Co-organisation of tutorials in the Grey group

May 2015	Co-organisation of the Grey group retreat
2013 - 2017	Webmaster for the group website of Pr. Clare Grey
July 2014	Organisation of the "Ion dynamics in confined systems" symposium at the University of Cambridge
2011 - 2013	Representative of staff on a fixed-term contract (PhD students, post-doctoral researchers, ATER, etc…) in the council of the PECSA laboratory
2010 - 2013	Installation and maintenance of a computer managing tool in the PECSA laboratory
Peer review	Reviewer for *ACS Nano, Nature Communications, Journal of Chemical Physics, Chemical Physics Letters, Electrochimica Acta, Journal of Physical Chemistry, Industrial & Engineering Chemistry Research, Journal of Power Sources, Journal of the Electrochemical Society, Electrochemistry Communications, Materials Horizons*

HONORS AND AWARDS

Prix Louis Armand 2018 – in Chemistry

Prize awarded by the French "Académie des Sciences" to a young French researcher, 30 years old at most, for a remarkable work in one of the following fields: applied mathematics, mechanics, physics, chemistry, biology and Earth sciences.

"ERC Starting Grant 2016"

Substantial funding for 5 years awarded to promising early career researchers to promote fundamental and independent research.

"Prix Solennel de la Chancellerie de Paris 2014, Arconati-Visconti"

Thesis award of 10 000 euros, given by the "Chancellerie des Universités de Paris", rewarding the excellence and the scientific and academic merits of a PhD thesis

"Darwin College Postdoctoral Research Associate"

Substantial association with "Darwin College" including an active participation in college life (formal dinners, seminars)

"Prix de thèse 2014 de la Division Chimie Physique"

Thesis award given by the Physical Chemistry Division (DCP) shared between the French Society of Chemistry (SCF) and the French Society of Physics (SFP)

Oppenheimer Research Fellowship, 2014

Three-year fellowship awarded by the School of Physical Sciences of the University of Cambridge (started on the 1st of October, 2014)

"Prix La Recherche", Physics

Prize from the French magazine "La Recherche"

Best Oral Presentation

Journées Francophones des Jeunes Physico-Chimistes, Dinard, France, 2012

Best Poster

Ionic Liquids: Faraday Discussion 154, Belfast, United Kingdom, 2011

Best Poster

ISEE'Cap 2011, Poznan, Poland, 2011

"Prix de l'Association"

Chimie ParisTech Alumni prize

PUBLICATIONS

31. "Computational insights into charge storage mechanisms of supercapacitors"
K. Xu, H. Shao, Z. Lin, C. Merlet, G. Feng, J. Zhu, P .Simon, *Energy & Environmental Materials*, **3**, 235 (2020)

30. "Effects of functional groups and anion size on the charging mechanism in layered electrode materials"
K. Xu, C. Merlet, Z. Lin, H. Shao, P.-L. Taberna, L. Miao, J. Jiang, J. Zhu, P .Simon, *Energy Storage Mater.*, **33**, 460 (2020)

29. "Local distortions and dynamics in hydrated Y-doped $BaZrO_3$"
A.Torayev, L. Sperrin, M. A. Gomez, J. Kattirtzi, C. Merlet, C. P. Grey, J. *Phys. Chem. C*, **124**, 16689 (2020)

28. "Efficient prediction of Nucleus Independent Chemical Shifts for polycyclic aromatic hydrocarbons"
D. Kilymis, A. P. Bartók, C. J. Pickard, A. C. Forse, C. Merlet, *Phys. Chem. Chem. Phys*, **22**, 13746 (2020)

27. "Ionic liquids under confinement: From systematic variations of the ion and pore sizes towards an understanding of the structure and dynamics in complex porous carbons"
E. H. Lahrar, A. Belhboub, P.Simon, C. Merlet, *ACS Appl. Mater. Inter.*, **12**, 1789 (2020)

26. "Carbons with regular pore geometry yield fundamental insights into supercapacitor charge storage"
Y. M. Liu, C. Merlet, B. Smit, *ACS Central Science*, **5**, 1813 (2019)

25. "On the development of an original mesoscopic model to predict the capacitive properties of carbon-carbon supercapacitors"
A. Belhboub, E. H. Lahrar, P. Simon, C. Merlet, *Electrochim. Acta*, **327**, 135022 (2019)

24. "Text-mining assisted review of the literature on Li-O_2 batteries"
A. Torayev, P. C. M. M. Magusin, C. P. Grey, C. Merlet, A. A. Franco, *J. Phys. Mater.*, **2**, 044004 (2019)

23. "On the importance of incorporating explicit 3D-resolved electrode mesostructures in Li-O_2 models"
A. Torayev, P. C. M. M. Magusin, C. P. Grey, C. Merlet, A. A. Franco, *ACS Appl. Energy Mater.*, **1**, 6433 (2018)

22. "Towards an atomistic understanding of disordered carbon electrode materials"
V. L. Deringer, C. Merlet, Y. Hu, T. H. Lee, J. A. Kattirtzi, O. Pecher, G. Csányi, S. R. Elliott, C. P. Grey , *Chem. Commun.*, **54**, 5988 (2018)

21. "Stochasticity of pores interconnectivity in Li-O_2 batteries and its impact on the variations in electrochemical performance"
A. Torayev, A. Rucci, P. C. M. M. Magusin, A. Demortière, V. De Andrade, C. P. Grey, C. Merlet, A. A. Franco, *J. Phys. Chem. Lett.*, **9**, 791 (2018)

20. "Structural characterization of the Li-ion battery cathode materials $LiTi_xMn_{2-x}O_4$ ($0.2 \leq x \leq 1.5$): A combined experimental ^{7}Li NMR and first-principles study"
R. Pigliapochi, I. D. Seymour, C. Merlet, A. J. Pell, D. T. Murphy, S. Schmid, C. P. Grey, *Chem. Mater.*, **30**, 817 (2018)

19. "Tracking ionic rearrangements and interpreting dynamic volumetric changes in two-dimensional metal carbide supercapacitors: A molecular dynamics simulations study"
K. Xu, Z. Lin, C. Merlet, P.-L. Taberna, L. Miao, J. Jiang, P. Simon, *ChemSusChem*, **11**, 1892 (2018)

18. "Direct observation of ion dynamics in supercapacitor electrodes using *in situ* diffusion NMR spectroscopy"
A. C. Forse, J. M. Griffin, C. Merlet, J. Carretero-González, A.-R. O. Raji, N. M. Trease, C. P. Grey, *Nature Ener.,* **2**, 16216 (2017)

17. "New perspectives on the charging mechanisms of supercapacitors"
A. C. Forse, C. Merlet, J. M. Griffin, C. P. Grey, *J. Am. Chem. Soc.,* **138**, 5731 (2016)

16. "New insights into the structure of nanoporous carbons from NMR, Raman and pair distribution function analysis"
A. C. Forse, C. Merlet, P. K. Allan, E. K. Humphreys, J. M. Griffin, M. Aslan, M. Zeiger, V. Presser, Y. Gogotsi, C. P. Grey, *Chem. Mater.,* **27**, 6848 (2015)

15. "NMR study of ion dynamics and charge storage in ionic liquid supercapacitors"
A. C. Forse, J. M. Griffin, C. Merlet, P. M. Bayley, H. Wang, P. Simon, C. P. Grey, *J. Am. Chem. Soc.*, **137**, 7231 (2015)

14. "Lattice simulation method to model diffusion and NMR spectra in porous materials"
C. Merlet, A. C. Forse, J. M. Griffin, D. Frenkel, C. P. Grey, *J. Chem. Phys,* **142**, 094701 (2015)

13. "Single electrode capacitances of porous carbons in neat ionic liquid electrolyte at 100°C: a combined experimental and modeling approach"
C. Péan, B. Daffos, C. Merlet, B. Rotenberg, P.-L. Taberna, P. Simon, M. Salanne, *J. Electrochem. Soc.*, **162**, A5091 (2015)

12. "The electric double layer has a life of its own"
C. Merlet, D. T. Limmer, M. Salanne, R. van Roij, P. A. Madden, D. Chandler, B. Rotenberg, *J. Phys. Chem. C,* **118**, 18291 (2014)

11. "On the dynamics of charging in nanoporous carbon-based supercapacitors"
C. Péan, C. Merlet, B. Rotenberg, P. A. Madden, P.-L. Taberna, B. Daffos, M. Salanne, P. Simon *ACS Nano, **8**,* 1576 (2014)

10. "Highly confined ions store charge more efficiently in supercapacitors"
C. Merlet, C. Péan, B. Rotenberg, P. A. Madden, B. Daffos, P.-L. Taberna, P. Simon, M. Salanne, *Nat. Commun,* **4**, 2701 (2013)

9. "Charge fluctuations in nanoscale capacitors"
D. T. Limmer, C. Merlet, M. Salanne, D. Chandler, P. A. Madden, R. van Roij, B. Rotenberg, *Phys. Rev. Lett.*, **111**, 106102 (2013)

8. "Computer simulations of ionic liquids at electrochemical interfaces"
C. Merlet, B. Rotenberg, P. A. Madden and M. Salanne, *Phys. Chem. Chem. Phys.,* **15**, 15781 (2013)

7. "Influence of solvation on the structural and capacitive properties of electrical double layer capacitors"
C. Merlet, M. Salanne, B. Rotenberg and P. A. Madden, *Electrochim. Acta*, **101**, 262 (2013)

6. "Simulating supercapacitors: Can we model electrodes as constant charge surfaces"
C. Merlet, C. Péan, B. Rotenberg, P. A. Madden, P. Simon, M. Salanne, *J. Phys. Chem. Lett.*, **4**, 264 (2013)

5. "New coarse-grained models of imidazolium ionic liquids for bulk and interfacial molecular simulations"
C. Merlet, M. Salanne and B. Rotenberg, *J. Phys. Chem. C*, **116**, 7687 (2012)

4. "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 Mat.*, **11**, 306 (2012)

3. "Imidazolium ionic liquid interfaces with vapor and graphite: Interfacial tension and capacitance from coarse-grained molecular simulations"
C. Merlet, M. Salanne, B. Rotenberg, P. A. Madden, *J. Phys. Chem. C*, **115**, 16613 (2011)

2. "Thermal conductivity of ionic systems from equilibrium molecular dynamics"
M. Salanne, D. Marrocchelli, C. Merlet, N. Ohtori and P. A. Madden, *J. Phys.: Condens. Matter*, **23**, 102101 (2011)

1. "Internal mobilities and diffusion in an ionic liquid mixture"
C. Merlet, P. A. Madden and M. Salanne, *Phys. Chem. Chem. Phys.*, **12**, 14109 (2010)

BOOK CHAPTERS

2. "Molecular dynamics simulations of electrochemical energy storage devices"
D. Marrocchelli, C. Merlet and M. Salanne, *Physical multiscale modeling and numerical simulations of electrochemical devices for energy conversion and storage – From theory to engineering practice*, Ed. A. A. Franco, M.-L. Doublet, W. Bessler, Springer (2016)

1. "The electrode – ionic liquid interface: a molecular point of view"
C. Merlet, M. Salanne, P. A. Madden, B. Rotenberg, *Electrostatics of Soft and Disordered Matter*, **p. 155**, Ed. D. S. Dean, J. Dobnikar, A. Naji, R. Podgornik, Pan Stanford Publishing, Singapore (2013)

PRESENTATIONS (#Poster, *Oral, **Invited oral)

2020

"*SuPERPORES, Structure-PErformance Relationships in PORous carbons for Energy Storage*", C. Merlet
** *IndTech2020, Digital Conference on Industrial Technologies, Visioconférence, October*

"*Computational investigation of high power devices*", C. Merlet (talk given online)
** *1st German-French summer workshop on high power devices, Jena, Germany, September*

"*On the development of a computationally efficient model to predict the performance of porous carbons as electrode materials for electrochemical capacitors*", A. Belhboub, E. H. Lahrar, P. Simon, C. Merlet
 # 71st Annual Meeting of the ISE, Online conference, September

"*Understanding and predicting the electrochemical properties of carbon / electrolyte interfaces in supercapacitors using multi-scale models*", C. Merlet,
** Seminar, ENS Lyon, France, January

2019

"Exploring the properties of concentrated electrolyte / electrode interfaces in supercapacitors using idealised coarse-grained models", C. Merlet,
** Seminar, The University of Bonn, Germany, December
** Heraeus Seminar: Operando surface science – Atomistic insights into electrified solid / liquid interfaces, Bad Honnef, Germany, December

"Precise structural characterisation of pure ionic liquids at carbon surfaces via molecular simulations", E. H. Lahrar, W.-Y. Tsai, N. Balke, P. Simon, C. Merlet
* ILMAT5 – International Conference on Ionic Liquid Based Materials, Paris, France, November

"Simulation of NMR spectra for molecules or ions diffusing in porous disordered carbons", C. Merlet, D. Kilymis, A. P. Bartók, C. J. Pickard, D. Frenkel, C. Grey
* Molecular and materials simulation at the turn of the decade: Celebrating 50 years of CECAM, Lausanne, Suisse, September

"On the development of a computationally efficient lattice model to predict the performance of carbon-carbon supercapacitors", E. H. Lahrar, A. Belhboub, C. Merlet
** Electrochemical energy storage: Theory meets industry, ECAM workshop, Paris, France, June

2018

"Exploring the structural and dynamical properties of concentrated electrolytes / electrode interfaces in supercapacitors using idealised coarse-grained models", E. H. Lahrar, A. Belhboub, C. Merlet
* Matériaux 2018, Strasbourg, France, November

"Investigating the properties of the electrode-electrolyte interface in porous carbon based supercapacitors using idealised coarse-grained models", E. H. Lahrar, A. Belhboub, C. Merlet
** RCTF2018, Toulouse, France, October

"Charge storage mechanisms and ion dynamics in nanoporous carbons for energy storage", C. Merlet
** 4th UK InterPore Conference, Aberdeen, United Kingdom, September

"NMR spectra calculations at the Daan scale", C. Merlet
** Scientific workshop honoring the 70th birthday of Prof. Daan Frenkel, Baiona, Spain, July

"Investigating the properties of the electrode-electrolyte interface in porous carbon based supercapacitors using idealised coarse-grained models", C. Merlet
** Seminar, EPFL, Sion, Switzerland, June

"Combining NMR, DFT calculations and coarse-grained models to improve the characterisation of energy storage materials", C. Merlet
** Seminar, Montpellier, France, June

"Multi-scale models to study dynamics and confinement in nanoporous carbons for energy storage applications", C. Merlet, E. H. Lahrar, A. Belhboub
** Journées Théorie, Modélisation et Simulation – JTMS2018, Paris, France, May

"Exploring the structural and dynamical properties of concentrated electrolytes / solid interfaces using idealised coarse-grained models", E. H. Lahrar, A. Belhboub, C. Merlet
** Electrostatics in Concentrated Electrolytes, CECAM workshop, Lausanne, Switzerland, March

2017

"Insights from simulations on the charge storage mechanisms and ion dynamics in nanoporous carbons for energy storage", C. Merlet
** RFCT, Journée Annuelle du Pôle Ouest, Nantes, France, November

"Étudier la dynamique et le confinement des ions dans les supercondensateurs par des simulations", C. Merlet
* TouCAM 2017, Toulouse, France, November

"Multi-scale models to study dynamics and confinement in nanoporous carbons for energy storage applications", C. Merlet
** CESEP'17, Lyon, France, October

"Combining NMR and simulations to probe charge storage mechanisms and ion dynamics in porous carbons for energy storage", C. Merlet, A. C. Forse, J. M. Griffin, D. Frenkel, C. P. Grey
** Understanding ionic liquids on different length and time scales, Leiden, The Netherlands, February

2016

"NMR study of charge storage mechanisms and ion dynamics in supercapacitors", C. Merlet, A. C. Forse, J. M. Griffin, D. Frenkel, C. P. Grey
** Multi-scale materials under the nanoscope, Paris, France, December

"Energy storage: Probing ion dynamics at the nanoscale in supercapacitors", C. Merlet, A. C. Forse, J. M. Griffin, D. Frenkel, C. P. Grey
** Darwin Lunch Seminar, Cambridge, Royaume-Uni, November

"Multi-scale models to study dynamics and confinement in materials for energy storage applications: From the molecular scale to the experimental scale", C. Merlet, M. Salanne, B. Rotenberg, P. A. Madden, D. Frenkel, C. P. Grey
** Seminar, Université de Bordeaux, Bordeaux, France, October
** Seminar, Université d'Orléans, Orléans, France, October
** Seminar, Université Paul Sabatier, Toulouse, France, September

"Lattice simulations and NMR in electrochemical systems: Including dynamic processes in NMR spectra prediction", C. Merlet, A. C. Forse, J. M. Griffin, I. D. Seymour, D. Frenkel and C. P. Grey
Future of Chemical Physics, Oxford, United Kingdom, August-September

"Development of original lattice simulations to include dynamic processes in NMR spectra prediction", C. Merlet, A. C. Forse, J. M. Griffin, I. D. Seymour, D. Frenkel and C. P. Grey
* Developments and Applications of Solid State NMR to Materials Science, Chemistry and Engineering Conference, Varna, Bulgaria, May

2015

"Lattice simulations and NMR in energy storage materials: Including dynamics in NMR spectra prediction", C. Merlet, A. C. Forse, J. M. Griffin, I. D. Seymour, D. Frenkel and C. P. Grey
** EMN meeting on computation and theory, Istanbul, Turkey, October

"NMR study of the electrode/electrolyte interface in supercapacitors", C. Merlet, A. C. Forse, J. M. Griffin, D. Frenkel and C. P. Grey
** COST action meeting, Ionic liquids at interfaces, Belek, Turkey, October

“Development of a new simulation method to model diffusion and NMR spectra in porous carbons: Insights into ion adsorption in supercapacitors”, C. Merlet, A. C. Forse, J. M. Griffin, D. Frenkel, C. P. Grey
** ISEE'Cap 2015, Montpellier, France, June
* SCF'15, Lille, France, July

“Development of a new simulation method to model diffusion and NMR spectra in porous carbons”, C. Merlet, A. C. Forse, J. M. Griffin, D. Frenkel, C. P. Grey
* STFC Early Career Researchers Conference 2015, Abingdon, United Kingdom, March

2014

“Study of the electrode/electrolyte interface in supercapacitors: insights from molecular simulations and NMR spectra prediction”, C. Merlet, B. Rotenberg, P. A. Madden, M. Salanne, D. Frenkel, C. P. Grey
** Workshop: Interfacial and transport properties of ionic liquids, Santiago de Compostela, Spain, November

“Energy storage: Understanding supercapacitors for improving them”, C. Merlet, B. Rotenberg, P. A. Madden, M. Salanne, D. Frenkel, C. P. Grey
** Darwin Lunch Seminar, Cambridge, United Kingdom, November

“Modélisation de l'adsorption des ions dans les carbones nanoporeux”, C. Merlet, B. Rotenberg, P. A. Madden, M. Salanne
** Journées Francophones des Jeunes Physicochimistes (JFJPC15), Dammarie-les-Lys, France, October

“Development of an original lattice simulation method to study the solid-liquid interface in porous materials”, C. Merlet, A. C. Forse, J. M. Griffin, D. Frenkel, C. P. Grey
Journées Francophones des Jeunes Physicochimistes (JFJPC15), Dammarie-les-Lys, France, October

“Development of a new lattice method to study dynamics processes in paramagnetic battery materials: the case of $Li_{1-x}MnO_2$”, C. Merlet, I. Seymour, D. Middlemiss, D. Frenkel, C. P. Grey
Paramagnetic NMR conference and workshop, Cambridge, United Kingdom, September

“Investigation of supercapacitors through an original lattice simulation method combined with in situ NMR experiments”, C. Merlet, A. C. Forse, J. M. Griffin, D. Frenkel, C. P. Grey
* 65th Annual Meeting of the ISE, Lausanne, Switzerland, September
** Modelling Ionic Liquids at Electrochemical Interfaces, CECAM workshop, Paris, France, August
# Carbon in Electrochemistry: Faraday Discussion 172, Sheffield, United Kingdom, July

"Étude de l'interface électrode/électrolyte dans les supercondensateurs : modélisation moléculaire et simulation de spectres RMN ", C. Merlet, M. Salanne, B. Rotenberg, P. A. Madden, D. Frenkel, C. P. Grey
** Seminar, Université Paul Sabatier, Toulouse, France, September

2013

"Charge fluctuations in nano-scale capacitors", C. Merlet, D. Limmer, M. Salanne, D. Chandler, P. A. Madden, R. van Roij, B. Rotenberg
* Modelling Ionic Liquids at Electrochemical Interfaces, CECAM workshop, Paris, France, September

"Stockage de charge dans les carbones nanoporeux : l'origine moléculaire de la super-capacité", C. Merlet, M. Salanne, B. Rotenberg, P. A. Madden
** 22ème Congrès Général de la SFP, Marseille, France, July

"Influence of confinement and solvation on the properties of supercapacitors: A molecular dynamics study", C. Merlet, M. Salanne, B. Rotenberg, P. A. Madden
* ISEE'Cap 2013, Taormina, Sicily, June

"Modeling electrode/electrolyte interfaces in supercapacitor systems", C. Merlet, M. Salanne, B. Rotenberg, P. A. Madden
** Symposium on Ionic Liquids, Oxford, United Kingdom, March
** Seminar, University of Oxford, United Kingdom, January

"Modélisation moléculaire de l'adsorption des ions aux interfaces carbone-électrolyte dans les supercondensateurs", C. Merlet, M. Salanne, B. Rotenberg, P. A. Madden
** 4ème Journée Batterie Lithium Ile de France, Thiais, France, September
* Journées d'Électrochimie 2013, Paris, France, July
* 2èmes Journées de l'Association Française de l'Adsorption, Paris, France, February

2012

"Comprendre le mécanisme de charge des supercondensateurs grâce à la dynamique moléculaire", C. Merlet, M. Salanne, B. Rotenberg, P. A. Madden, P.-L. Taberna, P. Simon, Y. Gogotsi
* Journées Modélisation à Paris, Paris, France, June
* Journées Francophones des Jeunes Physico-Chimistes, Dinard, France, October

"Understanding the Charging Mechanism of Nanoporous Carbon Electrodes from Molecular Dynamics Simulations", C. Merlet, M. Salanne, B. Rotenberg, P. A. Madden, P.-L. Taberna, P. Simon, Y. Gogotsi
*11th Spring Meeting of the ISE, Washington DC, USA, May
* 63rd Annual Meeting of the ISE, Prague, Czech Republic, August

2011

"Insights on Capacitive and Structural properties of [BMI][PF_6] Confined Between Graphite Electrodes from Molecular Dynamics", C. Merlet, M. Salanne, B. Rotenberg and P. A. Madden
Ionic Liquids: Faraday Discussion 154, Belfast, United Kingdom, August
ISEE'Cap 2011, Poznan, Poland, June