

MERLET Céline
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Post-doctoral researcher at the University of Cambridge
Darwin College Postdoctoral Research Associate

RESEARCH EXPERIENCE

October 2013 – Present

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 characterisations 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 **18 publications**
Author of **2 book chapters**
(A complete list of my publications is provided at the end of this document.)

Conferences Author of **30 talks** and **6 posters** given in national or international conferences, including **8 invited talks** in international conferences
(A complete list of my presentations is provided at the end of this document.)

TEACHING EXPERIENCE AND SUPERVISION

Since 2016 Co-supervision of the PhD project of Amangeldi Torayev, co-directed by Pr. C. Grey at the University of Cambridge and Pr. A. Franco at Université Picardie Jules Verne

2015 Supervision of the master thesis project of Amangeldi Torayev from February to August 2015, student of the MESC Master (Materials for Energy Storage and Conversion)

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

Since 2016 Organisation of tutorials in the Grey group

May 2015 Organisation of the Grey group retreat

Since 2013 Webmaster for the group website of Pr. Clare Grey

July 2013 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*, *Chemical Physics Letters*, *Electrochimica Acta*, *Journal of Physical Chemistry*, *Journal of Chemical Physics*, *Industrial & Engineering Chemistry Research*, *Journal of Power Sources*

HONORS AND AWARDS

“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

LANGUAGES/COMPUTER SCIENCE

French	Mother tongue
English	Fluent
Spanish	Fair working knowledge
Computer skills	Programming in C, fortran LaTeX, Xmgrace, Word, Excel, Power Point, VMD, Modeller, AMBER, Whatif, Gaussian Using HPC facilities (JADE and CURIE machines in France, HECTOR machine in the UK)

PUBLICATIONS

1. “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).

2. “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)

3. “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).

4. “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)

5. “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).

6. “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).

7. “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).

8. “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).

9. “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).

10. “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).

11. “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).

12. “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).

13. “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).

14. “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).

15. “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).

16. “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)

17. “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).

18. “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

19. “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).

20. “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)

2017

“Combining NMR and simulations to probe charge storage mechanisms and ion dynamics in porous carbons for energy storage”, C. Merlet, A. C. Forse, J. 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. 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. 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

** Séminaire, Université de Bordeaux, Bordeaux, France, October

** Séminaire, Université d’Orléans, Orléans, France, October

** Séminaire, 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 $\text{Li}_{1-x}\text{MnO}_2$ ”*, 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, 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][PF₆] 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