MATHIEU SALANNE
Assistant professor
Laboratoire PECSA
Université Pierre and Marie Curie (Paris, France)
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Curriculum Vitæ

June 2012 Habilitation degree, Université Pierre and Marie Curie : Modeling molten salts and ionic liquids for energy applications

November 2010 Visiting researcher, Universidade Federal de São Paulo

March 2010 Visiting researcher, Niigata University

Since September 2007 Assistant Professor, Université Pierre and Marie Curie

January 2007 – August 2007 Postdoctoral fellow, Institut de Physique Nucléaire : Electrochemical study of the grouped extraction of lanthanides in the molten salt LiF-ThF_4

2004–2006 Ph.D. thesis in condensed matter, Université Pierre and Marie Curie : Molecular simulation of high temperature molten fluorides

2001–2004 Master of engineering, Chimie Paristech

2003 Trainee in nuclear engineering, Massachusetts Institute of Technology : Removal of enriched boric acid from the primary coolant of reactors

Teaching

- Electrochemistry and physical chemistry, Université Pierre and Marie Curie (192 hours per year)
- Co-organizer of 3 tutorials on molecular simulations for young researchers

Fellowships & Award

2007 Colaureate of the award of the French magazine *La Recherche*, for the research work carried on the molecular simulation for the nuclear industry of the future

2005 2 months stay in the University of Edinburgh sponsored by the HPC-Europa program

Publications & Communications

PEER-REVIEWED ARTICLES

[1] **M. Salanne**, D. Marrocchelli, G.W. Watson, A cooperative mechanism for the diffusion of Li^+ ions in $LiMgSO_4F$, **J. Phys. Chem. C**, in press.

[2] S. Tazi, B. Rotenberg, **M. Salanne**, M. Sprik and M. Sulpizi, Absolute acidity of clay edge sites from ab-initio simulations, **Geochim. Cosmochim. Acta**, in press.

[3] C. Merlet, **M. Salanne** and B. Rotenberg, New coarse-grained models of imidazolium ionic liquids for bulk and interfacial molecular simulations, **J. Phys. Chem. C**, 116, 7687–7693 (2012).

[4] S. Tazi, A. Botan, **M. Salanne**, V. Marry, P. Turq and B. Rotenberg, Diffusion coefficient and shear viscosity of rigid water models, **J. Phys. : Condens. Matter**, 24, 284117 (2012).

[5] C. Merlet, B. Rotenberg, P.A. Madden, P.-L. Taberna, P. Simon, Y. Gogotsi and **M. Salanne**, On the molecular origin of supercapacitance in nanoporous carbon electrodes, **Nature Mater.**, 11, 306–310 (2012).

[6] S. Tazi, J.J. Molina, B. Rotenberg, P. Turq, R. Vuilleumier and **M. Salanne**, A transferable *ab initio* based force field for aqueous ions, **J. Chem. Phys.**, 136, 114507 (2012).

[7] **M. Salanne**, B. Rotenberg, S. Jahn, R. Vuilleumier, C. Simon and P.A. Madden, Including many-body effects in models for ionic liquids, **Theor. Chem. Acc.**, 131, 1143 (2012).

[8] **M. Salanne**, L.A.J. Siqueira, A.P. Seitsonen, P.A. Madden and B. Kirchner, From molten salts to room temperature ionic liquids : Simulation studies on chloroaluminate systems, **Faraday Discuss.**, 154, 171–188 (2012).

[9] A.-L. Rollet, **M. Salanne** and H. Groult, Structural effects on the electrical conductivity of molten fluorides : Comparison between LiF-YF_3 and LiF-NaF-ZrF_4, **J. Fluorine Chem.**, 134, 44–48 (2012).

[10] J.J. Molina, J.-F. Dufrêche, **M. Salanne**, O. Bernard and P. Turq, Primitive models of ions in solution from molecular descriptions : A perturbation approach, **J. Chem. Phys.**, 135, 234509 (2011).

[11] **M. Salanne** and P.A. Madden, Polarization effects in ionic solids and melts, **Mol. Phys.**, 109, 2299–2315 (2011) – invited review article.

[12] C. Merlet, **M. Salanne**, B. Rotenberg and P.A. Madden, Imidazolium Ionic Liquid Interfaces with Vapor and Graphite : Interfacial Tension and Capacitance from Coarse-Grained Molecular Simulations, **J. Phys. Chem. C**, 115, 16613–16618 (2011).

[13] O. Pauvert, **M. Salanne**, D. Zanghi, C. Simon, S. Reguer, D. Thiaudière, Y. Okamoto, H. Matsuura and C. Bessada, Ion Specific Effects on the Structure of Molten AF-ZrF_4 Systems (A^+ = Li^+, Na^+, and K^+), **J. Phys. Chem. B**, 115, 9160–9167 (2011).

[14] **M. Salanne**, C. Simon and P.A. Madden, Optical basicity scales in protic solvents : water, hydrogen fluoride, ammonia and their mixtures, **Phys. Chem. Chem. Phys.**, 13, 6305–6308 (2011).

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

[16] J.J. Molina, S. Lectez, S. Tazi, **M. Salanne**, J.-F. Dufrêche, J. Roques, E. Simoni, P.A. Madden and P. Turq, Ions in solutions : Determining their polarizabilities from first-principles, **J. Chem. Phys.**, 134, 014511 (2011.)

[17] C. Merlet, P.A. Madden and **M. Salanne**, Internal mobilities and diffusion in an ionic liquid mixture, **Phys. Chem. Chem. Phys.**, 12, 14109–14114 (2010).

[18] S. Tazi, **M. Salanne**, C. Simon, P. Turq, M. Pounds and P.A. Madden, Potential-induced ordering transition of the adsorbed layer at the ionic liquid / electrified metal interface, **J. Phys. Chem. B**, 114, 8453–8459 (2010).

[19] O. Pauvert, D. Zanghi, **M. Salanne**, C. Simon, A. Rakhmatullin, H. Matsuura, Y. Okamoto, F. Vivet and C. Bessada, In situ experimental evidence for a nonmonotonous structural evolution with composition in the molten LiF-ZrF_4 system, **J. Phys. Chem. B**, 114, 6472–6479 (2010).

[20] B. Rotenberg, **M. Salanne**, C. Simon and R. Vuilleumier, From localized orbitals to material properties : building classical force fields for nonmetallic condensed matter systems, **Phys. Rev. Lett.**, 104, 138301 (2010).

[21] D. Marrocchelli, **M. Salanne** and P.A. Madden, High-pressure behaviour of GeO_2 : a simulation study, **J. Phys. : Condens. Matter**, 22, 152102 (2010).

[22] J.J. Molina, J.-F. Dufrêche, **M. Salanne**, O. Bernard, M. Jardat and P. Turq, Models of electrolyte solutions from molecular descriptions : the example of NaCl solutions, **Phys. Rev. E**, 80, 065103 (2009).

[23] V. Sarou-Kanian, A.-L. Rollet, **M. Salanne**, C. Simon, C. Bessada and P.A. Madden, Diffusion coefficients and local structure in basic molten fluorides : *in situ* NMR measurements and molecular dynamics simulations, **Phys. Chem. Chem. Phys.**, 11, 11501–11506 (2009).

[24] M. Pounds, S. Tazi, **M. Salanne** and P.A. Madden, Ion adsorption at a metallic electrode : an *ab initio*-based simulation study, **J. Phys : Condens. Matter**, 21, 424109 (2009).

[25] O. Benes, P. Zeller, **M. Salanne** and R.J.M. Konings, Density functional theory, molecular dynamics, and differential scanning calorimetry study of the RbF-CsF phase diagram, **J. Chem. Phys.**, 130, 134716 (2009).

[26] N. Ohtori, **M. Salanne** et P.A. Madden, Calculations of the thermal conductivities of ionic materials by simulation with polarizable interaction potentials, **J. Chem. Phys.**, 130, 104507 (2009).

[27] D. Marrocchelli, **M. Salanne**, P.A. Madden, C. Simon and P. Turq, The construction of a reliable potential for GeO_2 from first principles, **Mol. Phys.**, 107, 443–452 (2009).

[28] **M. Salanne**, C. Simon, H. Groult, F. Lantelme, T. Goto et A. Barhoun, Transport in molten LiF-NaF-ZrF_4 mixtures : a combined computational and experimental approach, **J. Fluorine Chem.**, 130, 61–66 (2009).

[29] **M. Salanne**, C. Simon, P. Turq et P.A. Madden, Heat-transport properties of molten fluorides : determination from first-principles, **J. Fluorine Chem.**, 130, 38–44 (2009).

[30] **M. Salanne**, R. Vuilleumier, P.A. Madden, C. Simon, P. Turq et B. Guillot, Polarizabilities of individual molecules and ions in liquids from first principles, **J. Phys. : Condens. Matter**, 20, 494207 (2008).

[31] **M. Salanne**, C. Simon, P. Turq et P.A. Madden, Intermediate range chemical ordering of cations in simple molten alkali halides, **J. Phys. : Condens. Matter**, 20, 332101 (2008).

[32] **M. Salanne**, C. Simon, P. Turq et P.A. Madden, Calculation of activities of ions in molten salts with potential application to the pyroprocessing of nuclear waste, **J. Phys. Chem. B**, 112, 1177–1183 (2008).

[33] **M. Salanne**, C. Simon, P. Turq et P.A. Madden, Conductivity-viscosity-structure : unpicking the relationship in an ionic liquid, **J. Phys. Chem. B**, 111, 4678–4684 (2007).

[34] **M. Salanne**, C. Simon, P. Turq and P.A. Madden, Simulation of the liquid-vapor interface of molten $LiBeF_3$, **C. R. Chim.**, 10, 1131–1136 (2007).

[35] H. Groult, F. Lantelme, **M. Salanne**, C. Simon, C. Belhomme, B. Morel and F. Nicolas, Role of elemental fluorine in nuclear field, **J. Fluorine Chem.**, 128, 285–295 (2007).

[36] **M. Salanne**, C. Simon et P. Turq, Molecular dynamics simulation of hydrogen fluoride mixtures with 1-ethyl-3-methylimidazolium fluoride : dynamic features, **J. New. Mat. Electrochem. Systems**, 9, 291-295 (2006).

[37] **M. Salanne**, C. Simon, P. Turq, R.J. Heaton et P.A. Madden, A first-principles description of liquid BeF_2 and its mixtures with LiF : 2. Network formation in LiF-BeF_2, **J. Phys. Chem. B**, 110, 11461–11467 (2006).

[38] R.J. Heaton, R. Brookes, P.A. Madden, **M. Salanne**, C. Simon et P. Turq, A first-principles description of liquid BeF_2 and its mixtures with LiF : 1. Potential development and pure BeF_2, **J. Phys. Chem. B**, 110, 11454–11460 (2006).

[39] **M. Salanne**, C. Simon et P. Turq, Molecular dynamics simulation of hydrogen fluoride mixtures with 1-ethyl-3-methylimidazolium fluoride : a simple model for the study of structural features, **J. Phys. Chem. B**, 110, 3504-3510 (2006).

NON PEER-REVIEWED INVITED REVIEW ARTICLES

[40] A.-L. Rollet and **M. Salanne**, Studies of the local structures of molten metal halides, **Annu. Rep. Prog. Chem., Sect. C : Phys. Chem.**, 107, 88–123 (2011).

Oral communications

INTERNATIONAL CONFERENCES AND WORKSHOPS

June 2012 Workshop Ionic Liquids and Coulomb Fluids at Interfaces, Windsor Great Park (United Kingdom), **invited talk**,Understanding the charging mechanism of nanoporous carbon electrodes from molecular dynamics simulations, **M. Salanne**, C. Merlet, B. Rotenberg, P.A. Madden, P.-L. Taberna, P. Simon and Y. Gogotsi.

May 2012 11th spring meeting of the International Society of Electrochemistry, Washington (USA), Building polarizable force fields for lithium fluorophosphate materials, **M. Salanne** and D. Marrocchelli.

August 2011 International Conference on Solution Chemistry, La Grande Motte, **invited talk**, Lewis basicity scales in liquids from first-principles, **M. Salanne** and C. Simon.

August 2011 Faraday Discussion 154 : Ionic liquids, Belfast (United Kingdom), From molten salts to RTILs : Simulation studies on chloroaluminate systems, **M. Salanne**, L.A.J. Siqueira, A.P. Seitsonen, P.A. Madden and B. Kirchner.

June 2011 9^{th} International Symposium on Molten Salts Chemistry & Technology, Trondheim (Norway), Molten Salts : From first-principles to material properties, **M. Salanne**, P.A. Madden and C. Simon.

December 2010 Transient Chemical Structures in Dense Media, Paris, **invited talk**, Chemistry of molten fluorides from first-principles, **M. Salanne**, P.A. Madden, C. Simon and P.A. Madden.

November 2010 Mini-symposium on Molecular Simulation, São Paulo (Brazil), From Localized Orbitals to Material Properties : Wannier Orbitals Force Field, **M. Salanne**, B. Rotenberg, C. Simon, R. Vuilleumier.

October 2010 Nuclear Materials Conference (NUMAT 2010), Karlsruhe (Allemagne), Prediction of Thermal Properties of Molten Salts from Computer Simulations, **M. Salanne**, C. Simon, N. Ohtori and P.A. Madden.

June 2010 CECAM workshop : Advances in the Implementation of Polarizable Force Fields for Molecular Simulations, Lausanne (suisse), **invited talk**, Computing condensed-phase polarizabilities of individual molecules and ions, **M. Salanne**.

March 2010 EUCHEM Conference on Molten Salts and Ionic Liquids, Bamberg (Germany), Interface between an ionic liquid and a metallic electrode : an *ab initio*-based simulation study, **M. Salanne**, M. Pounds, S. Tazi, P.A. Madden, C. Simon and P. Turq.

April 2009 CECAM workshop : Computational models of RTIL, Dublin (Ireland), **invited talk**, Molten salts : building interaction potentials from first-principles, **M. Salanne**.

June 2008 7^{th} Liquid Matter Conference, Lund (Sweden), Molten salts : from first-principles to material properties, **M. Salanne**, C. Simon, P. Turq and P.A. Madden.

September 2005 7^{th} International Symposium on Molten Salts Chemistry & Technology, Toulouse (France), Molecular dynamics simulation of hydrogen fluoride mixtures with imidazolium fluorides, **M. Salanne**, C. Simon and P. Turq.

NATIONAL CONFERENCES AND WORKSHOPS

March 2011 Matériaux and Fluides Haute Température (MFHT 4), Orléans, Ionic liquids : From first-principles to material properties, **M. Salanne**, P.A. Madden , C. Simon and N. Ohtori.

August 2010 Journées Matière Condensée, Paris, Des orbitales localisées aux propriétés des matériaux, **M. Salanne**, B. Rotenberg, C. Simon, R. Vuilleumier.

June 2010 Atelier du GNR PARIS X-Ray absorption, Avignon, Determining the structure of molten salts from a coupled XAFS/NMR/molecular dynamics approach, **M. Salanne**.

February 2010 Journées du PCR Applications Nucléaires des Sels Fondus, Paris, Simulation de l'interface électrode / sel fondu par dynamique moléculaire, S. Tazi, **M. Salanne**, M. Pounds, C. Simon and P.A. Madden.

June 2009 Journées modélisation de l'ENS-ENSCP, Paris, Thermal conductivities of molten salts, **M. Salanne**, C. Simon, N. Ohtori and P.A. Madden.

February 2009 Journées du PCR Réacteur à Sels Fondus, Paris, Propriétés physico-chimiques de LiF-ThF_4 : calculs de dynamique moléculaire, **M. Salanne**, C. Simon, P. Turq and P.A. Madden.

June 2008 Journées modélisation de l'ENS-ENSCP, Paris, Détermination de polarisabilités ioniques et moléculaires dans les liquides, **M. Salanne**, C. Simon, P. Turq, P.A. Madden and R. Vuilleumier.

February 2008 Journées du PCR Réacteur à Sels Fondus, Paris, Propriétés physico-chimiques des sels fondus : approche couplée simulation / expérience, **M. Salanne**, C. Simon, P. Turq, H. Groult, T. Goto and P.A. Madden.

February 2008 Workshop SiMaDes II, Grenoble, Ionic systems : from first-principles to material properties, **M. Salanne**, C. Simon, P. Turq and P.A. Madden.

February 2008 Journées du GDR PARIS 2008, Avignon, Coefficients d'activité dans les sels fondus par dynamique moléculaire, **M. Salanne**, C. Simon and P. Turq.

January 2008 Atelier du GDR PARIS Redox and Actinides, Orsay, Simulation des propriétés redox des sels fondus, **M. Salanne**, C. Simon, P. Turq, S. Reed, M. Pounds and P.A. Madden.

SEMINARS

June 2011 Département de chimie, University of Cambridge (United Kingdom), Simulations of ionic liquids for energy applications

November 2010 Laboratoire des matériaux hybrides, Université Fédérale de São Paulo (Brazil), Study of the ionic liquid // metallic electrode interface by molecular dynamics simulations

March 2010 Département de chimie, Université de Niigata (Japan), Molten salts : from first-principles to material properties

October 2010 Institut Français du Pétrole, Rueil-Malmaison, Simulation des liquides ioniques

January 2009 Laboratoire CEMHTI, Orléans, Sels fondus : des principes premiers aux propriétés des matériaux

June 2007 Institut de Physique Nucléaire, Orsay, Étude des sels fondus : électrochimie and simulation numérique