

**Benjamin Rotenberg**  
né le 14 février 1982 à Paris, marié  
ResearcherID : C-5490-2014 / ORCID : 0000-0001-5198-4650

Laboratoire PHENIX, Sorbonne Université  
4 pl. Jussieu, 75005 Paris  
benjamin.rotenberg@sorbonne-universite.fr

## Situation actuelle

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**Directeur de Recherche CNRS** en section 13 (Chimie Physique, théorique, analytique)

Co-responsable de l'équipe Modélisation et Expériences Multiéchelles depuis 2019.

Laboratoire Physicochimie des électrolytes, et nanosystèmes interfaciaux - UMR 8234 CNRS Sorbonne Université.

**Mots clés** : simulations moléculaires et mésoscopiques, coarse-graining, phénomènes électrocinétiques, interfaces et milieux poreux chargés, nanofluidique, argiles, supercondensateurs, énergie bleue, bruit électrique dans les électrolytes...

## Formation

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**2012 Habilitation à Diriger des Recherches**

*Physicochimie des interfaces chargées : modélisation multi-échelles et applications pour l'énergie*

**2004 – 2007 Thèse Modélisation multi-échelle du comportement de l'eau et des ions dans les argiles**

sous la direction de Pierre Turq à l'Université Pierre et Marie Curie financement de l'Andra.

**2003 – 2004 DEA en Matière Condensée : Chimie et Organisation, UPMC (Très Bien, rang 1<sup>er</sup>)**

**2001 – 2005** Cursus de chimie à l'**Ecole Normale Supérieure** (Paris)

## Expérience professionnelle

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(Co-)direction de **9 thèses, co-encadrement de 4 autres thèses et 12 post-docs**, encadrement de L3, M1 et M2.

**2023 Visiting Researcher** à l'Université de Tel Aviv (Israël), dans le groupe de David Andelman.

**2019 & 2020 Visiting Researcher** à UC Berkeley, Californie (USA), dans le groupe de David Limmer.

**Depuis 2018 Directeur de Recherche CNRS**

**2018 Visiting Researcher** au Helmholtz-Zentrum Berlin (Allemagne), dans le groupe de Joachim Dzubiella.

**2010 & 2011 Professeur invité** à l'Université de Barcelone (Espagne), dans le groupe d'Ignacio Pagonabarraga.

**2010, 2011 & 2013 Visiting Scholar** à UC Berkeley, Californie (USA), dans le groupe de David Chandler.

**2008 – 2018 Chargé de Recherche CNRS** (CR2, puis CR1 en 2013) Laboratoire PECSA, PHENIX depuis 2014.

**2007 – 2008 Post-doc** à l'institut AMOLF, Amsterdam (Pays-Bas), avec Daan Frenkel.

**2004 – 2007 Thèse** au Laboratoire Liquides Ioniques et Interfaces Chargées sous la direction de Pierre Turq.

**2004** Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Golm (Allemagne), avec Markus Antonietti.

**2003** Laboratoire Colloïdes et Matériaux Divisés, ESPCI, avec Jérôme Bibette.

**2003** Department of theoretical chemistry, Cambridge (Royaume-Uni), avec Jean-Pierre Hansen.

## Distinctions

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**2021** Co-lauréat du **Prix spécial Joseph Fourier (GENCI-Atos)** pour le code MetalWalls

**2020** Membre de la promotion "**Cadres à haut potentiel 2020**" du CNRS

**2018 HPCwire Readers' & Editors' Choice** (best use of High Performance Computing in Energy)

**2017 Friedrich-Wilhelm Bessel Research Award** de la **Alexander von Humboldt Foundation** (Allemagne).

**2015 Médaille de Bronze du CNRS.**

**2014** Sélectionné par la New York Academy of Sciences pour participer au **Science and Technology in Society (STS) Forum**, Kyoto, dans le cadre du « Future Leaders program ».

**2013-2018 Membre Distingué Junior** de la Société Chimique de France.

**2013 Grand Prix Michel Guillaud Schlumberger** de l'Académie des Sciences.

**2013** Co-lauréat du **Prix La Recherche 2013**, mention « Physique ».

**2013 Prix Jeune Chercheur** de la Division de Chimie Physique (commune à la SCF et la SFP).

**2012-2017 Prime d'Excellence Scientifique** du CNRS.

**2011** Young Faculty poster prize, **Mini Statistical Mechanics Meeting** (Berkeley, Californie, USA).

**2007** Co-lauréat du **Prix La Recherche 2007**, mention « Énergie ».

**2001** Admis à l'**École Normale Supérieure** (Paris, rang 1<sup>er</sup>) et à l'**École Polytechnique** (1<sup>er</sup>).

**2000** Médaille de bronze aux **Olympiades Internationales de Chimie** (Copenhague, Danemark).

## Enseignement

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**2018 Ecole internationale SJSACMS** (Bangalore, Inde) : mesoscopic hydrodynamics, Lattice-Boltzmann (doct.).  
**Depuis 2015 Ecole internationale PISACMS** (Paris) : mesoscopic hydrodynamics, Lattice-Boltzmann (M2/doct.).  
**2015 Ecole MeMoSim** (Lyon) : méthodes probabilistes pour systèmes complexes (DCP, ANF CNRS).  
**2015 – 2018 Master Chimie Physique Analytique et Théorique** (UPMC) : modélisation de la solvatation (M1).  
**2010 & 2011 Master in Computational Physics** (Barcelone) : modélisation multi-échelle (M2).  
**Depuis 2009 Master Chimie Physique Analytique et Théorique** (UPMC) : modélisation multi-échelle (M2).  
**2009 – 2017 International Master in Advanced Clay Science** (Poitiers) : modélisation moléculaire (M1).  
**2005 – 2007 Moniteur en Chimie** (UPMC).  
**Examinateur Oral de chimie au concours d'entrée à l'ENS** (2012-2014)

## Partenariats et financement de projets

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**H2020 Porteur** du projet **ERC Consolidator SENSES** (1.8M€, 2020-25)  
*Hôte* de la **Marie Curie Fellowship** Molecular Control de Sophie Marbach, avec NYU (2020-2023)  
*Principal Investigator* du réseau européen **FET-OPEN NANOPHLOW** (total 3.3M€, 2018-21)  
*Coordinateur adjoint* du réseau européen **ETN NANOTRANS** (total 3.9M€, 2016-20)  
*Participant* à l'action **COST NMR Relaxometry** (2016-20)

**FP7 Membre associé** des réseaux européens **ITN COMPLOIDS** (2009-13) et **Euratom CATCLAY** (2010-14)

**RS2E Membre** du Réseau sur le Stockage Electrochimique de l'Energie

**ANR Principal Investigator** du projet ANR **DIADEM** (2022-25) – 650k€  
*Principal Investigator* du projet ANR-DFG **NEPTUNE** (2017-21) – 390k€  
*Porteur* du projet JCJC **LENNS** (2015-19) – 180k€  
*Co-direction* avec Pierre Turq du projet **SIMISOL** (2009-12) – 300k€  
*Partenaire* des projets **MAICANANO** (2010-13), **CELADYCT** (2012-16) et **BALWISE** (2019-23)

**Ville de Paris Porteur** du projet Emergence(s) "Energie bleue et désalinisation" (2016-19) – 250k€

**IFP-En** Thèses d'Alexandru Botan (2008-11) et Pauline Simonnin (2014-17) – 200k€

**Andra** Post-doc de Magali Duvail (2010-11) et thèse d'Amaël Obliger (2011-14) – 175k€

**DIM Oxymore** de la Région Ile-de-France, avec Anne Boutin : thèse de Wilfried Louisfrema (2013-16) – 100k€

**France-Berkeley Fund Principal Investigator** avec D. Chandler (2012-13, 10k\$) et D. Limmer (2018-19, 11k\$)

**GNR PARIS Porteur** d'un projet (2010-11) – 3.5k€

**GENCI Porteur** de projets – 6 millions (2016) et 1,8 millions (2017) d'heures de calcul sur Curie ; 600.000 heures sur Curie et 700.000 heures sur Irene (2017) ; 2 millions (2018) et 3.5 millions (2019) d'heures sur Occigen ; 33.500 (2021) et 30.000 (2022) heures GPU sur Jean Zay.

**ISCD Partenaire** de l'équipe-projet **MAESTRO** de l'ISCD, Alliance Sorbonne Université (depuis 2020).

## Responsabilités collectives et administration de la recherche

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**UMR PHENIX** Co-responsable de l'équipe Modélisation et Expériences Multi-échelles depuis 2019, responsable du site web ([www.phenix.cnrs.fr](http://www.phenix.cnrs.fr)) depuis 2009. Ancien CSSI (Correspondant de Sécurité des Systèmes d'Information) [2013-2020] et ancien membre du conseil de l'UMR [2009-2010].

**Programme NEEDS** (Nucléaire : Energie, Environnement, Déchets, Société) du CNRS : co-direction du Projet Fédérateur "Milieux Poreux" [2012-2018].

**CNRS** Dans le cadre de la promotion 2020 des "cadres à haut potentiel", préparation d'un rapport sur la mission d'expertise du CNRS, ayant contribué à la mise en place en 2022 de la Mission Pour l'Expertise Scientifique.

**UPMC** Chargé de mission (vice-présidence recherche et innovation) sur la participation de l'UPMC au programme européen JOPRAD "Toward a joint programming on radioactive waste disposal" [2016-2018].

**UFR 926** (UFR 926) Membre élu du conseil et du conseil scientifique, membre nommé de la commission des personnels IATOS [2009-2013]. Comités de sélection Maître de Conférences et ATER.

**iMAT** Membre du CoDir de l'Institut de science des matériaux de l'Alliance Sorbonne Université [Depuis 2022]

**Labex MATISSE** Membre [2011-2017] puis co-animateur [2015-2017] du comité de pilotage de l'axe transversal "Modélisation Multi-échelle".

**Andra** Comité de pilotage du groupement de laboratoires "Transferts" [2009-2014].

**Subatech** Membre invité du Conseil scientifique du laboratoire [2019].

**DIM RESPORE** Correspondant pour le laboratoire PHENIX [depuis 2017].

**GDR NAME** Correspondant pour le laboratoire PHENIX et membre du GT Stockage de l'énergie [depuis 2020].

**Evaluateur** ERC, ANR, PRACE (HPC Europe), Swiss National Science Foundation (Suisse), Netherlands Organisation for Scientific Research NWO et Technology Foundation STW (Pays-Bas), Foundation for Polish Science FNP (Pologne), Croatian Science Foundation (Croatie), Slovenian Research Agency (Slovénie), Programme Emergences (Ville de Paris), Labex Chammatt, I-SITE E2S, Comité ECOS Nord, Université Franco-Allemande.

**Membre de jury ou rapporteur** **26 thèses** (Paris, Orsay, Pau, Clermont-Ferrand, Marne-la-Vallée, Grenoble, Toulouse, Montpellier, Barcelone, Cambridge, Lund) et **6 HDR** (Paris, Lyon, Nantes, Clermont-Ferrand, Prague)

## Animation scientifique

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**Membre de l'Editorial Board** de *Molecular Physics* et guest editor de 3 volumes de cette revue.

**Reviewer** (~20/an) pour *Nature Commun.*, *Nature Phys.*, *PNAS*, *Phys. Rev. Lett.*, *Phys. Rev. X*, *J. Phys. Chem. Lett.*, *J. Chem. Phys.*, *J. Phys. Chem.*, *J. Chem. Theory Comput.*, *Soft Matter*, *ACS Nano*, *Sci. Rep.*, *Langmuir*, *Europhys. Lett.*, *Nanolett.*, *J. Power Sources*, *Mol. Phys.*, *J. Coll. Interf. Sci.*, *Phys. Rev. E*, *J. Phys. Condens. Matter*, *Geochim. Cosmochim. Acta*, *Oil & Gas Sci. Technol.*, *Int. J. Greenh. Gas Control*, *Adv. Water Resour.*, ...

**Membre du bureau** de la sub-division *Modélisation et Simulation* et **membre du Conseil** de la *Division de Chimie Physique* commune à la Société Chimique de France et à la Société Française de Physique [2015-2018].

## Organisation de conférences

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**Juillet 2022** CECAM Conference *New frontiers in liquid matter* à Paris

**Juin 2022** CECAM Workshop *Atomistic simulations of interfacial processes in energy materials* à Paris

**Avril 2022** CECAM Workshop *Numerical Techniques for Nonequilibrium Steady States* à Mainz, Allemagne

**Mai 2021** CECAM Workshop *Digital Prequel - Numerical Techniques for Nonequilibrium Steady States* (online)

**Janvier 2020** Meeting en l'honneur de Loup Verlet à Paris.

**Mai 2018** Journée Théorie, Modélisation et Simulation de la DCP, à Paris

**Avril 2018** CECAM Workshop *Phoretic effects at the nanoscale* à Lausanne, Suisse

**Mars 2018** CECAM Workshop *Electrostatics in Concentrated Electrolytes* à Lausanne, Suisse

**Juin 2017** CECAM School *Transport of soft matter at the nanoscale* à Mainz, Allemagne

**Avril 2017** CECAM Workshop *Exploiting finite-size effects in simulations*, Paris

**Décembre 2016** Workshop annuel du *GDRI Multiscale Materials Under the Nanoscope (M2UN)*

**Décembre 2016** Journées annuelles de *NEEDS - Milieux Poreux*

**Juillet 2016** CECAM-FR-MOSER Meeting *Algorithms and codes for the simulation of explicit electrodes*

**Décembre 2015** Journées annuelles de *NEEDS - Milieux Poreux*

**Juin 2015** Comité Scientifique de *LowPerm2015* à Rueil-Malmaison.

**Mai 2015** CECAM Workshop *Simulation of systems under thermodynamic-like gradients* à Saragosse, Espagne.

**Décembre 2014** Journées annuelles de *NEEDS - Milieux Poreux*

**Octobre 2014** Premier Colloque *NEEDS*, Nantes.

**Août 2014** CECAM Workshop *Modelling ionic liquids at electrochemical interfaces* à Paris.

**Juillet 2014** Meeting en l'honneur de Pierre Turq à Paris.

**Mars 2014** CFCAM Discussion Meeting *Simulation of systems under thermodynamic gradients* à Paris.

**Décembre 2013** Meeting en l'honneur de Jean-Pierre Hansen à Paris.

**Novembre 2013** Journées annuelles de *NEEDS - Milieux Poreux* à Paris.

**Septembre 2013** CFCAM Discussion Meeting, *Modelling ionic liquids at electrochemical interfaces* à Paris

**Décembre 2012** Colloque de lancement du programme *NEEDS - Milieux Poreux* à Paris.

**Octobre 2012** Session Molecular Modelling au *International Symposium "Using Natural and Engineered Clay-based Barriers for the Containment of Radioactive Waste"* à Montpellier.

**Juin 2011** CECAM Workshop *Microscopic-Scale View of CO<sub>2</sub> Sequestration* à Lausanne, Suisse.

**Mai 2011** CECAM Workshop *New Challenges for the Simulation of Electrokinetic Phenomena* à Paris.

## Publications et communications

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**138 articles** dont 1 *Chem. Rev.*, 1 *Nature Materials*, 3 *Nature Communications*, 1 *Nature Energy*, 1 *Ann. Rev. Phys. Chem.*, 2 *PNAS*, 1 *ACS Nano*, 2 *JACS*, 1 *Phys. Rev. X*, 6 *Phys. Rev. Lett.*, 1 *Angew. Chem. Int. Ed.*, 1 *ACS Cent. Sci.*, 2 *J. Phys. Chem. Lett.* (dont 1 perspective), 2 *J. Chem. Theory Comput.*, 1 *Soft Matter*, 3 *Faraday Discussions* (dont 1 cover), 20 *J. Phys. Chem. B&C* (dont 1 cover), 26 *J. Chem. Phys.* (dont 1 perspective), 5 *PCCP* (dont 2 perspectives), 3 *Geochim. Cosmochim. Acta*, 2 *Energy Storage Materials*

**7 actes de congrès avec comité de lecture**

**6 chapitres d'ouvrages**

**44 conférences invitées (dont 5 keynotes)**

**15 autres communications orales** et **18 posters** à des conférences

**39 séminaires invités** et **24 autres communications**

## Liste des publications

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### REVUES INTERNATIONALES AVEC COMITÉ DE LECTURE

- [1] B. Rotenberg, R. Taïeb, V. Vénard et A. Maquet,  $H_2^+$  in intense laser field pulses : ionization versus dissociation within moving nuclei simulations, *J. Phys. B* **35**, L397-L402 (2002).
- [2] A. Moncho-Jorda, B. Rotenberg et A.A. Louis, Effect of polymer-polymer interactions on the surface tension of colloid-polymer mixtures, *J. Chem. Phys.* **119**, 12667-12672 (2003).
- [3] B. Rotenberg, J. Dzubiella, J.-P. Hansen et A.A. Louis, Thermodynamic perturbation theory of the phase behavior of colloid / interacting polymer mixtures, *Mol. Phys.* **102**, 1-11 (2004).
- [4] V. Krakoviack, B. Rotenberg et J.-P. Hansen, An integral equation approach to effective interactions between polymers in solution, *J. Phys. Chem. B* **108**, 6697-6706 (2004).
- [5] S. Mandal, N. Lequeux, B. Rotenberg, M. Tramier, J. Fattaccioli, J. Bibette et B. Dubertret, Encapsulation of magnetic and fluorescent nanoparticles in emulsion droplets, *Langmuir* **21**, 4175-4179 (2005).
- [6] B. Rotenberg, A. Cadène, J.-F. Dufrêche, S. Durand-Vidal, J.-C. Badot et P. Turq, An analytical model for probing ion dynamics in clays with Broadband Dielectric Spectroscopy, *J. Phys. Chem. B* **109**, 15548-15557 (2005).
- [7] B. Rotenberg, J.-F. Dufrêche, et P. Turq, Frequency-dependent dielectric permittivity of salt-free charged lamellar systems, *J. Chem. Phys.* **123**, 154902-154913 (2005).
- [8] D. Zerrouki, B. Rotenberg, S. Abramson, J. Baudry, C. Goubault, F.L. Calderon, D. Pine et J. Bibette, Preparation of doublet, triangular, and tetrahedral colloidal clusters by controlled emulsification, *Langmuir* **22**, 57-62 (2006).
- [9] B. Rotenberg, J.-F. Dufrêche, B. Bagchi, E. Giffaut, J.-P. Hansen et P. Turq, Ion dynamics in compacted clays : Derivation of a two-state diffusion-reaction scheme from the lattice Fokker-Planck equation, *J. Chem. Phys.* **124**, 154701-154712 (2006).
- [10] D. Moroni, B. Rotenberg, J.-P. Hansen, S. Succi, et S. Melchionna, Solving the Fokker-Planck kinetic equation on a lattice, *Phys. Rev. E* **73**, 066607 (2006).
- [11] B. Rotenberg et D. Moroni, Second-order lattice Fokker-Planck algorithm from the trapezoidal rule, *Phys. Rev. E* **74**, 037701 (2006).
- [12] B. Rotenberg, V. Marry, J.-F. Dufrêche, E. Giffaut et P. Turq, A multiscale approach to ion diffusion in clays : Building a two-state diffusion-reaction scheme from microscopic dynamics, *J. Coll. and Interf. Sci.* **309**, 289-295 (2007).
- [13] B. Rotenberg, V. Marry, R. Vuilleumier, N. Malikova, C. Simon et P. Turq, Water and ions in clays : Unraveling the interlayer/micropore exchange using molecular dynamics, *Geochimica et Cosmochimica Acta* **71**, 5089-5101 (2007).
- [14] B. Rotenberg, V. Marry, J.-F. Dufrêche, N. Malikova, E. Giffaut et P. Turq, Modeling water and ion diffusion in clays : A multiscale approach, *Comptes Rendus Chimie* **10**, 1108-1116 (2007).
- [15] V. Marry, B. Rotenberg et P. Turq, Structure and dynamics of water at a clay surface from molecular dynamics simulation, *Phys. Chem. Chem. Phys.* **10**, 4802-4813 (2008).

- [16] B. Rotenberg, I. Pagonabarraga et D. Frenkel, Dispersion of charged tracers in charged porous media, *Europhys. Lett.* **83**, 34004 (2008).
- [17] M. Jardat, J.-F. Dufrêche, V. Marry, B. Rotenberg et P. Turq Salt exclusion in charged porous media : A coarse-graining strategy in the case of montmorillonite clays, *Phys. Chem. Chem. Phys.*, **11**, 2023-2033 (2009).
- [18] B. Rotenberg, J.-P. Morel, V. Marry, P. Turq et N. Morel-Desrosiers, On the driving force of cation exchange in clays : Insights from combined microcalorimetry experiments and molecular simulations, *Geochimica et Cosmochimica Acta*, **73**, 4034-4044 (2009).
- [19] B. Rotenberg, I. Pagonabarraga et D. Frenkel, Coarse-grained simulations of charge, current and flow in heterogeneous media, *Faraday Discussions*, **144**, 223-243 (2010). Cet article fait la **couverture du volume "Multiscale Modelling of Soft Matter"**.
- [20] N. Malikova, E. Dubois, V. Marry, B. Rotenberg et P. Turq, Dynamics in clays - combining neutron scattering and microscopic simulation, *Z. Phys. Chem*, **244**, 153-181 (2010).
- [21] B. Rotenberg, M. Salanne, C. Simon et R. Vuilleumier, From localized orbitals to material properties : Building classical force fields for nonmetallic condensed matter systems, *Phys. Rev. Lett.*, **104**, 138301 (2010).
- [22] B. Rotenberg, V. Marry, N. Malikova et P. Turq, Molecular simulation of aqueous solutions at clays surfaces, *J. Phys. Cond. Matt.*, **22** 284114 (2010).
- [23] I. Pagonabarraga, B. Rotenberg et D. Frenkel, Recent advances in the modelling and simulation of electrokinetic effects : bridging the gap between atomistic and macroscopic descriptions (Perspective Article), *Phys. Chem. Chem. Phys.*, **12**, 9566 (2010).
- [24] A. Botan, B. Rotenberg, V. Marry, P. Turq et B. Noetinger, Carbon Dioxide in Montmorillonite Clay Hydrates : Thermodynamics, Structure, and Transport from Molecular Simulation, *J. Phys. Chem. C*, **114**, 14962 (2010).
- [25] A. Botan, B. Rotenberg, V. Marry, P. Turq et B. Noetinger, Hydrodynamics in clay nanopores, *J. Phys. Chem. C*, **115**, 16109 (2011).
- [26] C. Merlet, M. Salanne, B. Rotenberg et 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 (2011).
- [27] B. Rotenberg, A.J. Patel et D. Chandler, Molecular explanation for why talc surfaces can be both hydrophilic and hydrophobic, *J. Am. Chem. Soc.*, **133**, 20521 (2011).
- [28] M. Salanne, B. Rotenberg, S. Jahn, R. Vuilleumier, C. Simon et P.A. Madden, Including many-body effects in models for ionic liquids, *Theo. Chem. Acc.*, **131**, 1143 (2012).
- [29] S. Tazi, J. Molina, B. Rotenberg, P. Turq, R. Vuilleumier et M. Salanne, A transferable ab-initio based force field for aqueous ions, *J. Chem. Phys.*, **136**, 114507 (2012).
- [30] C. Merlet, B. Rotenberg, P.A. Madden, P.-L. Taberna, P. Simon, Y. Gogotsi et M. Salanne, On the molecular origin of supercapacitance in nanoporous carbon electrodes, *Nature Mater.*, **11**, 306 (2012).
- [31] C. Merlet, M. Salanne et B. Rotenberg, New Coarse-Grained Models of Imidazolium Ionic Liquids for Bulk and Interfacial Molecular Simulations *J. Phys. Chem. B*, **116**, 7687 (2012).
- [32] S. Tazi, A. Botan, M. Salanne, V. Marry, P. Turq et B. Rotenberg, Diffusion coefficient and shear viscosity of rigid water models, *J. Phys. Cond. Matt.*, **24**, 284117 (2012).
- [33] S. Tazi, B. Rotenberg, M. Salanne, M. Sprik and M. Sulpizi, Absolute acidity of clay edge sites from ab-initio simulations, *Geochimica et Cosmochimica Acta*, **94**, 1 (2012).
- [34] M. Levesque, O. Bénichou, R. Voituriez and B. Rotenberg, Taylor Dispersion with Adsorption and Desorption, *Phys. Rev. E*, **86**, 036316 (2012).
- [35] M. Levesque, V. Marry, B. Rotenberg, G. Jeanmairet, R. Vuilleumier and D. Borgis, Solvation of Complex Surfaces via Molecular Density Functional Theory, *J. Chem. Phys.*, **137**, 224107 (2012).
- [36] C. Merlet, C. Péan, B. Rotenberg, P.A. Madden, P. Simon et M. Salanne, Simulating Supercapacitors : Can We Model Electrodes as Constant Charge Surfaces ? *J. Phys. Chem. Lett.*, **4**, 264 (2013).
- [37] A. Botan, V. Marry, B. Rotenberg, P. Turq et B. Noetinger, How Electrostatics Influences Hydrodynamic Boundary Conditions : Poiseuille and Electro-Osmotic Flows in Clay Nanopores, *J. Phys. Chem. C*, **117**, 978 (2013).
- [38] M. Levesque, O. Benichou et B. Rotenberg, Molecular diffusion between walls with adsorption and desorption, *J. Chem. Phys.*, **138**, 034107 (2013).
- [39] C. Merlet, M. Salanne, B. Rotenberg et P.A. Madden, Influence of solvation on the structural and capacitive properties of electrical double layer capacitors, *Electrochimica Acta*, **101**, 262 (2013).

- [40] B. Rotenberg et I. Pagonabarraga, Electrokinetics : insights from simulation on the microscopic scale (Topical Review), *Mol. Phys.*, **111**, 827 (2013).
- [41] M. Levesque, M. Duvail, I. Pagonabarraga, D. Frenkel et B. Rotenberg, Accounting for adsorption and desorption in Lattice-Boltzmann simulations, *Phys. Rev. E*, **88**, 013308 (2013).
- [42] A. Obliger, M. Duvail, M. Jardat, D. Coelho, S. Bekri et B. Rotenberg, Numerical homogenization of electrokinetic equations in porous media using Lattice-Boltzmann simulations, *Phys. Rev. E*, **88**, 013019 (2013).
- [43] D.T. Limmer, C. Merlet, M. Salanne, D. Chandler, P.A. Madden, R. van Roij et B. Rotenberg, Charge fluctuations in nano-scale capacitors *Phys. Rev. Lett.*, **111**, 106102 (2013).
- [44] C. Merlet, B. Rotenberg, P.A. Madden et M. Salanne, Computer simulations of ionic liquids at electrochemical interfaces (Perspective Article), *Phys. Chem. Chem. Phys.*, **15**, 15781 (2013).
- [45] A. Botan, V. Marry, B. Rotenberg, P. Turq et B. Noetinger, Correction to “How Electrostatics Influences Hydrodynamic Boundary Conditions : Poiseuille and Electro-Osmotic Flows in Clay Nanopores”, *J. Phys. Chem. C*, **117**, 20376 (2013).
- [46] C. Merlet, C. Péan, B. Rotenberg, P.A. Madden, B. Daffos, P.-L. Taberna, P. Simon et M. Salanne, Highly confined ions store charge more efficiently in supercapacitors, *Nature Comm.*, **4**, 2701 (2013).
- [47] L.M. Hamm, I.C. Bourg, A.F. Wallace et B. Rotenberg, Molecular Simulation of CO<sub>2</sub>- and CO<sub>3</sub>-Brine-Mineral Systems, *Rev. Mineral. Geochem.*, **77**, 189 (2013).
- [48] A. Carof, V. Marry, M. Salanne, J.-P. Hansen, P. Turq et B. Rotenberg, Coarse-graining the dynamics of nano-confined solutes : The case of ions in clays, *Mol. Simul.*, **40**, 237 (2013).
- [49] D. Borgis, R. Assaraf, B. Rotenberg et R. Vuilleumier, Computation of pair distribution functions and three-dimensional densities with a reduced variance principle, *Mol. Phys.*, **111**, 3486 (2013).
- [50] C. Péan, C. Merlet, B. Rotenberg, P.A. Madden, P.-L. Taberna, B. Daffos, M. Salanne et P. Simon, On the dynamics of charging in nanoporous carbon-based supercapacitors, *ACS Nano*, **8**, 1576 (2014).
- [51] A. Carof, R. Vuilleumier et B. Rotenberg, Two algorithms to compute projected correlation functions in molecular dynamics simulations, *J. Chem. Phys.*, **140**, 124103 (2014).
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- [20] *Science and Technology in Society (STS) Forum*, Kyoto, Japon [10/2014]. Participant in the « Future Leaders program ».

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- [29] **Keynote speaker**, *Goldschmidt 2017*, Paris [08/2017], Multiscale modeling of electrokinetic transport in porous materials, B Rotenberg.
- [30] **Keynote speaker**, *MIGRATION 17 : 16<sup>th</sup> International Conference on Chemistry and Migration Behaviour of Actinides and Fission Products in the Geosphere*, Barcelone, Espagne [09/2017]. Micro- and mesoscopic simulations of clay and cement-based materials, B. Rotenberg.
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- [37] *CECAM Workshop "Memory Effects in Dynamical Processes : Theory and Computational Implementation"*, online [06/2021]. Computing memory kernels from noise reconstruction by a deterministic approach, R. Vuilleumier and B. Rotenberg.
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- [41] *CECAM Workshop "Charged Species in Bulk and Interfaces : Transport and Regulation"*, Vienne, Autriche [09/2022]. Making Sense of Electrical Noise by Simulating Electrolyte Solutions, B. Rotenberg.

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- [43] *Nanofluidics at the crossroads*, Collège de France, Paris [05/2023]. Electrode/electrolyte interfaces : From electronic response to interfacial structure, dynamics and thermodynamics using classical MD simulations, B. Rotenberg.
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- [31] *Euroclay*, Paris [07/2019], **communication orale**, Mineral- and Ion-Specific Effects at Clay-Water Interfaces : Structure, Diffusion, and Hydrodynamics, B. Rotenberg, P. Simonnin, V. Marry, B. Noetinger et C. Nieto-Draghi
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- [33] *Faraday Discussions "Iontronics : from fundamentals to ion-controlled devices"*, Edimbourg, Royaume-Uni [06/2023], **communication orale**, Electrical noise in electrolytes : a theoretical perspective, B. Rotenberg, T. Hoang Ngoc Minh, J. Kim, G. Pireddu, I. Chubak, S. Nair.

## SÉMINAIRES

- [1] Département de chimie de l'université de Cambridge (Royaume-Uni) [02/2006]
- [2] Laboratoire Liquides Ioniques et Interfaces Chargées (UPMC) [04/2007]
- [3] FOM Institute for Atomic and Molecular Physics (Amsterdam, Pays-Bas) [11/2007]
- [4] CEA Saclay [02/2008]
- [5] Schlumberger Cambridge Research Center (Cambridge, Royaume-Uni) [10/2008]
- [6] FOM Institute for Atomic and Molecular Physics (Amsterdam, Pays-Bas) [10/2008]
- [7] Département de Physique de la Technische Universität de München (Allemagne) [07/2009]
- [8] Département de Chimie de l'Université de Californie, Berkeley [01/2010]
- [9] Département de Génie Chimique de l'Université de Californie, Berkeley [03/2010]
- [10] Département de Physique de l'Université de Barcelone, Espagne [06/2010]
- [11] Institut Français du Pétrole, Rueil-Malmaison [10/2010]
- [12] Département de Chimie de l'Université de Californie, Berkeley [01/2011]
- [13] Département de Physique de l'Université de Barcelone, Espagne [05/2011]
- [14] Ecole Normale Supérieure, Département de Chimie (Pôle de Physico-chimie Théorique) [06/2011]
- [15] IFP Energies Nouvelles, Rueil-Malmaison [09/2011]
- [16] Institut Paul Scherrer, Villigen, Suisse [10/2011]
- [17] BP Institute (Cambridge, Royaume-Uni) [11/2012]
- [18] Laboratoire Modélisation et Simulation Multi Echelle (Université Paris Est) [11/2013]
- [19] Académie des Sciences, Section Géosciences [11/2013]
- [20] MIT, Department of Civil and Environmental Engineering, (Cambridge, MA, Etats-Unis) [01/2014]
- [21] Institut des Sciences Moléculaires (Nouvelle Université de Bordeaux) [06/2014]
- [22] Département de Physique de l'Université de Rome "La Sapienza", Italie [09/2014]
- [23] Institute for Theoretical Physics, Université d'Utrecht, Pays-Bas [10/2014]
- [24] Institut Charles Gerhardt, Montpellier [11/2014]
- [25] Ecole Normale Supérieure, Département de Chimie (Pôle de Physico-chimie Théorique) [12/2014]
- [26] Ecole Normale Supérieure, Département de Physique [01/2016]
- [27] Université de Mainz, Département de Physique [01/2016]
- [28] Helmholtz-Zentrum Berlin für Materialien und Energie, Allemagne [10/2016]
- [29] Université Paris Diderot (séminaire SCAN) [12/2016]
- [30] IFP Energies Nouvelles, Rueil-Malmaison [06/2017]
- [31] Institut de Physique de Rennes [10/2017]
- [32] Université de Mainz, Département de Physique [11/2018]
- [33] Freie Universität Berlin, Département de Physique [12/2018]
- [34] Université de Bochum, Département de Chimie [11/2019]
- [35] Laboratoire Jacques-Louis Lions, Sorbonne Université [02/2020]
- [36] Duke University, Département de Chimie (en visio) [10/2020]
- [37] Freie Universität Berlin, Département de Physique [03/2022]
- [38] Korea Institute of Energy Technology (KENTECH, en visio) [04/2023]
- [39] Université de Stuttgart, Institute for Computational Physics [06/2023]

## AUTRES

- [1] Journées de modélisation de Paris centre (ENS-ENSCP) [05/2006]
- [2] Journée des doctorants du Groupe Français des Argiles (Ecole des Mines, Paris) [11/2006]
- [3] Journée commune des Groupements de Recherche PARIS et MOMAS (IHP, Paris) [03/2007]
- [4] Journée des doctorants de l'ANDRA (ENSCP) [06/2007]
- [5] Journée des doctorants de l'ANDRA (ENSCP) [06/2008]
- [6] Journée commune des GNR PARIS et MOMAS (Ecole Polytechnique) [03/2010]
- [7] Journées de modélisation de Paris centre (ENS-ENSCP) [06/2010]
- [8] Journée commune des GNR PARIS et MOMAS (Université Claude Bernard, Lyon) [11/2010]
- [9] Journée Modélisation en physicochimie pour le nucléaire (UPMC) [01/2011]
- [10] Journée de l'UMR PECSA, Paris [02/2011]
- [11] Comité de suivi des recherches sur l'aval du cycle (COSRAC, MESR, PARIS) [02/2013]
- [12] Journée des CR1 de l'Institut de Chimie (INC) du CNRS [06/2013]
- [13] Journée annuelle du LABEX MATISSE [06/2015]
- [14] Table ronde à la journée "Modélisation : succès et limites" (CNRS et Académie des Technologies) [12/2016]
- [15] Meeting annuel du réseau européen ETN NANOTRANS (Berlin) [02/2017]
- [16] Journée d'étude des liquides (Paris) [06/2018]
- [17] Réunion semestrielle du RS2E (Montpellier) [10/2018]
- [18] Rencontres prospectives du Réseau Français de Chimie Théorique (Nantes) [06/2019]
- [19] Meeting annuel du réseau européen ETN NANOTRANS (Barcelone) [02/2020]
- [20] Réunion semestrielle du RS2E (visio) [10/2020]
- [21] Journée de lancement du livre "Étonnante Chimie" organisée par l'INC (Paris) [09/2021]
- [22] CurieOsity, association des étudiants de physique de Sorbonne Université (Paris) [11/2021]
- [23] Échanges avec des lycéens autour du livre "Étonnante Chimie" et du grand oral du bac (Paris) [04/2022]
- [24] Conférence "Beaucoup de bruit pour rien ?" lors de la Nuit de l'ENS (Paris) [09/2022]