BENJAMIN ROTENBERG
born Feb. 14^{th} 1982 in Paris
married

Laboratoire PHENIX, Sorbonne Université
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Current position and research interests

CNRS senior researcher, 13^{th} section of CNRS (Physical Chemistry), since 2018 (researcher since 2008).
PHENIX Laboratory "Physical chemistry of electrolytes and interfacial nanosystems" CNRS & Sorbonne Université

Keywords : molecular and mescocopic simulations, coarse-graining, electrokinetic effects, interfaces, charged porous materials, nanofluidics, clays, supercapacitors, blue energy, electrical noise in electrolytes

Research activities

2018 Visiting Researcher in the group of Joachim Dzubiella. at Helmholtz-Zentrum Berlin, Germany.

2010, 2011 & 2013 Visiting Scholar in the group of David Chandler at the University of California, Berkeley.

2010 & 2011 Invited Professor in the group of Ignacio Pagonabarraga at the University of Barcelona, Spain.

2007 – 2008 Post-doctoral fellow AMOLF institute, Amsterdam, The Netherlands, with Daan Frenkel.

2004 – 2007 PhD at the Ionic Liquids and Charged Interfaces Laboratory, UPMC, with Pierre Turq.

2004 Max-Planck-Institut fur Kolloïd- und Grenzflächenforschung, Golm, Germany, with Markus Antonietti.

2003 Colloids and Divided Materials Laboratory, ESPCI, Paris, with Jérôme Bibette.

2003 Department of theoretical chemistry, Cambridge University, UK, with Jean-Pierre Hansen.

Education

2012 Habilitation à Diriger des Recherches

2004 – 2007 Ph. D at UPMC, on the Multiscale Modelling of water and ions in clays. Supervisor : Pr. Pierre Turq. Funding from the French nuclear waste management agency (Andra)

2001 – 2005 École Normale Supérieure (Paris). **Bsc** (2002) and **Msc** (2004) in Chemical Physics

Teaching

2012-2014 Examiner (chemistry oral examination) for the admission to École Normale Supérieure

2010 & 2011 Master in Computational Physics (Barcelona) : Multiscale Modelling and Simulations

Since 2009 Master in Physical, Analytical and Theoretical Chemistry at UPMC (Paris) : Multiscale Modelling

2009 – 2017 International Master in Advanced Clay Science (Poitiers) : Molecular Simulations

2005 – 2007 Teaching Assistant (chemistry) at Université Pierre et Marie Curie (Paris).

2004 Examiner (physics) in "classes préparatoires" at lycée Louis-le-Grand (Paris)

Distinctions

2021 Co-laureate of the **Special Prize Joseph Fourier (GENCI-Atos)** for the MetalWalls code

2020 Participant in the **High potential leaders** 2020 program of CNRS

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

2017 Friedrich-Wilhelm Bessel Research Award of the **Alexander von Humboldt Foundation** (Germany)

2015 Bronze Medal of CNRS

2014 Selected by the New York Academy of Sciences to participate in the **Science and Technology in Society (STS) Forum**, Kyoto, within the « Future Leaders program »

2013-2018 Junior Distinguished Member of the French Chemical Society.

2013 Grand Prix Michel Gouilloud Schlumberger of the French Academy of Sciences.

2013 Co-laureate of the **Prix La Recherche 2013**, in « Physics ».

2013 Young Researcher Prize of the Division de Chimie Physique (French Chemical and Physical Societies)

2012-2017 Award for Scientific Excellence from CNRS

2007 Co-laureate of the **Prix La Recherche 2007**, in « Energy »

2001 Ranked 1^{st} at the national entrance selection for both **École Normale Supérieure** and **École Polytechnique**

2000 Bronze medal at the International Chemistry Olympiads (Copenhagen, Denmark)

Publications and communications

126 articles including 1 *Nature Materials*, 2 *Nature Communications*, 1 *Nature Energy*, 1 *Ann. Rev. Phys. Chem.*, 1 *ACS Nano*, 2 *JACS*, 1 *Phys. Rev. X*, 5 *Phys. Rev. Lett.*, 1 *Angew. Chem. Int. Ed.*, 1 *ACS Cent. Sci.*, 2 *J. Phys. Chem. Lett. (including 1 perspective)*, 2 *J. Chem. Theory Comput.*, 1 *Soft Matter*, 1 *Faraday Discussion* (cover), 20 *J. Phys. Chem. B&C* (including 1 cover), 22 *J. Chem. Phys.*, 5 *PCCP* (including 2 perspectives), 3 *Geochim. Cosmochim. Acta*, 8 *Phys. Rev. E*, ...

7 peer-reviewed proceedings

6 book chapters

37 invited conferences (including 4 keynotes), 14 other oral presentations and **18 posters** at conferences

36 invited seminars and **21 other communications**

ARTICLES

[1] B. Rotenberg, R. Taïeb, V. Véniard 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). This paper made the **cover of the "Multiscale Modelling of Soft Matter" issue**.

[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).

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[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).

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[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).

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[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).

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[52] B. Rotenberg, Physicochimie des interfaces chargées : modélisation multi-échelle et applications pour l'énergie, *L'Actualité Chimique*, **384**, 21 (2014).

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[56] G. Jeanmairet, V. Marry, M. Levesque, B. Rotenberg et D. Borgis, Hydration of Clays at the Molecular Scale : The Promising Perspective of Classical Density Functional Theory, *Mol. Phys.*, **112**, 1320 (2014).

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[61] B. Rotenberg, V. Marry, M. Salanne, M. Jardat et P. Turq, Multiscale modelling of transport in clays, from the molecular to the sample scale, *C.R. Geoscience*, **346**, 298 (2014).

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[63] A. Carof, M. Salanne, T. Charpentier et B. Rotenberg, Accurate Quadrupolar NMR Relaxation Rates of Aqueous Cations from Classical Molecular Dynamics, *J. Phys. Chem. B*, **118**, 13252 (2014).

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

[65] J.-M. Vanson, F.-X. Coudert, B. Rotenberg, M. Levesque, C. Tardivat, M. Klotz and A. Boutin, Unexpected coupling between flow and adsorption in porous media, *Soft Matter*, **11**, 6125 (2015).

[66] W. Louisfrema, B. Rotenberg, F. Porcher, J.-L. Paillaud, P. Massiani and A. Boutin, Cation redistribution upon dehydration of $Na_{58}Y$ faujasite zeolite : a joint neutron diffraction and molecular simulation study, *Mol. Simul.*, **41**(16-17), 1371 (2015).

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[69] A. Botan, V. Marry and B. Rotenberg, Diffusion in bulk liquids : finite-size effects in anisotropic systems, *Mol. Phys.*, **113**(17-18), 2674 (2015).

[70] C. Péan, B. Daffos, B. Rotenberg, P. Levitz, M. Haefele, P.-L. Taberna, P. Simon, M. Salanne, Confinement, desolvation and electrosorption effects on the diffusion of ions in nanoporous carbon electrodes, *J. Am. Chem. Soc.*, **137**(39), 12627 (2015).

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[80] W. Louisfrema, J.-L. Paillaud, F. Porcher, E. Perrin, T. Onfroy, P. Massiani, A. Boutin, B. Rotenberg, Cation Migration and Structural Deformations upon Dehydration of Nickel-Exchanged NaY Zeolite : A Combined Neutron Diffraction and Monte Carlo Study, *J. Phys. Chem. C*, **120**, 18115 (2016).

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[89] T. Mendez-Morales, M. Burbano, M. Haeffele, B. Rotenberg and M. Salanne, Ion-ion correlations across and between electrified graphene layers, *J. Chem. Phys.*, **148**, 193812 (2018).

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[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 [10/2014]
[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 Materialen 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]

OTHERS

[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] Journées des CR1 de l'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]