

# José Antonio Gárate

PhD

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## Personal Info

Date of birth *29 of July 1983*

Place of birth *Santiago, Chile*

Nationality *Chilean-French*

Marital status *Married*

## Languages

Spanish *Native*

English *Advanced*

French *Basic*

German *Basic*

## Academic Experience

December 2017 - present **Young Research Scientist**, *Millennium Institute Interdisciplinary Center for Neuroscience*, Valparaíso, Chile.

March 2016 - present **Assistant Professor**, *Computational Biology Laboratory, Fundación Ciencia & Vida*, Santiago, Chile.

March 2013 - February 2016 **Post-Doc**, *Computational Biology Laboratory, Fundación Ciencia & Vida*, Santiago, Chile.

March 2011 - March 2013 **Post-Doc**, *Molecular Modelling and Simulation group (MMS), Universität für Bodenkultur Wien*.

2008-2010 **PhD**, *Material and Molecular Simulation Group, UCD School of Chemical and Bioprocess Engineering, University College Dublin*, Dublin, Ireland.

2005-2007 **Molecular Biotechnology Engineer**, *Universidad de Chile*, Santiago, Chile.

2002-2005 **Bachelor in Molecular Biotechnology Engineering**, *Universidad de Chile*, Santiago, Chile.

## Projects

2010 - 2020 **Millennium Institute Interdisciplinary Center for Neuroscience**, .  
Role **Investigator**.

2016 - 2019 **FONDECYT project 1160574**, *Is there a voltage-controlled hydraulic gating in the human Connexin 26 hemichannel?* .

- Role **Co-investigator.**
- 2012 - 2015 **FONDECYT Post-Doc project 3130547** , *Free Energy Calculations of Carbon-Nanotube assisted Water self-difussion.*
- Role **Principal Investigator.**
- 2013 - 2015 **PIA ACT-1107** , *Integration of structural biology in the development of bionanotechnology.* .
- Role **Investigator.**
- 2008 - 2017 **Proyecto de Financiamiento Basal PFB16**, *Fundación Ciencia & Vida* .
- Role **Young Researcher.**
- 2010 - 2012 **European Research Commission**, *Efficient and accurate simulation techniques for free energies, enthalpies and entropies* .
- Role **Post-Doc.**

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## PhD Thesis

- January 2008 **The influence of electric fields on nano and biosystems** .  
 December 2010
- Laboratory Material and Molecular Simulation Group, UCD School of Chemical and Bioprocess Engineering, University College Dublin
- Description Equilibrium and non-equilibrium Molecular Dynamics Simulations of nano and biosystems like carbon nanotubes, membrane channels and nanorods adsorbed on gold surfaces under the influence of electric fields.

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## Diploma Thesis

- March 2006 **A role for molecular dynamics in the modelling of biological**  
 May 2007 **macromolecules.**
- Laboratory Centre for Bioinformatics,CBUC, Faculty of Biological Sciences, Catholic University of Chile.
- Description The utility of molecular dynamics as an evaluation tool in the modeling of biological macromolecules.

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## Supervised Theses

- 2014-present **Mechanical and Chemical unfolding of knotted proteins.**  
 Gutierrez S.
- Laboratory Computational Biology Laboratory, Fundación Ciencia & Vida.  
 Duty PhD thesis co-supervisor
- 2014-present **Exploring the membrane potential of a simple dual membrane system by using a constant electric field.**  
 Escalona Y.
- Laboratory Computational Biology Laboratory, Fundación Ciencia & Vida.  
 Duty Master thesis co-supervisor
- 2013 **Shapes and Free Energies of Biopolymers,Computational Studies of Structure and Molecular Recognition.**  
 Nagy G.

- Laboratory Material and Molecular Simulation Group, UCD School of Chemical and Bioprocess Engineering, University College Dublin
- Duty PhD thesis Tutor
- 2013 **From model systems to biomolecular complexes. Exploring entropy and protein stability.**  
Lai B.
- Laboratory Material and Molecular Simulation Group, UCD School of Chemical and Bioprocess Engineering, University College Dublin
- Duty PhD thesis Tutor
- 2010 **Diffusion and interactions of carbon dioxide and oxygen in the vicinity of the active site of Rubisco: a molecular dynamics study.**  
O'Reilly S
- Laboratory Material and Molecular Simulation Group, UCD School of Chemical and Bioprocess Engineering, University College Dublin

## Teaching Experience

- January 2017 **International Course: Advanced Computational Methods in Drug Discovery (ACMD2)**, *Fundación Ciencia & Vida.*
- Rol Lecturer
- November 2015 **International Spring School: Applied Statistical Thermodynamics, from theory to molecular dynamics simulations**, *Fundación Ciencia & Vida.*
- Duty Course organizer and Lecturer
- July 2014 - present **Classical Statistical Thermodynamics**, *Fundación Ciencia & Vida.*
- Duty Course organizer and Lecturer
- April 2015 - present **Computational Biology**, *PhD program in Medical Sciences*, Universidad Católica.
- Duty Lecturer
- November 2014 - present **Bioinformatics**, *PhD program in Biotechnology*, Universidad Nacional Andrés Bello.
- Duty Lecturer
- 2011 - 2013 **Modelling and Simulation of Biomolecules**, *Master program*, Universität für Bodenkultur Wien.
- Duty Lecturer

## Peer Reviewed Publications

- 2017 Sebastian E. Gutierrez-Maldonado, **Jose Antonio Garate**, Maria Jose Retamal, Marcelo Cisternas, Ulrich G. Volkmann, Tomas Perez-Acle "*Accessing the structural and thermodynamic properties of ultra-thin layers of C32 adsorbed on a SiO<sub>2</sub> surface*" Chem. Phys. Lett, accepted (2017).
- 2017 F Villanelo, Y Escalona, C Pareja-Barrueto, **JA Garate**, IM Skerrett, T Perez-Acle "*Accessing gap-junction channel structure-function relationships through molecular modelling and simulations*" BMC Cell Biology, 18(Suppl 1):5 (2017).

- 2016 Niall J. English and **Jose Antonio Garate** "*Near-microsecond human aquaporin 4 gating dynamics in static and alternating external electric fields: Nonequilibrium molecular dynamics*" J. Chem. Phys, 145:085102 (2016).\*
- 2016 Marracino Paolo,Liberti Micaela, Trapani Erika, Burnham Christian J,Avena, Massimiliano,Garate, **José-Antonio**, Apollonio Francesca, English, Niall J "*Human Aquaporin 4 Gating Dynamics under Perpendicularly-Oriented Electric-Field Impulses: A Molecular Dynamics Study.*" IJMS, 1422-0067 (2016).
- 2016 Yerko Escalona, **Jose A. Garate**, Raul Araya-Secchi, Tien Huynh, Ruhong Zhou and Tomas Perez-Acle, "*Exploring the membrane potential of simple dual-membrane systems as models for Gap-junction channels.*" Biophys J. accepted (2016).
- 2016 **Jose Antonio Garate** and Tomas Perez-Acle "*From dimers to collective dipoles: Structure and dynamics of methanol/ethanol partition by narrow carbon nanotubes*" J. Chem. Phys, 144:6:064105 (2016).\*
- 2015 Yu Chong, Cuicui Ge1, Zaixing Yang1, **Jose Antonio Garate**, Zonglin Gu, Jeffrey K. Weber, Jiajia Liu, and Ruhong Zhou "*Reduced cytotoxicity of graphene nanosheets mediated by blood-protein coating*" ACS Nano, 9;6:5713-5724 (2015).
- 2015 Guangxing Duan, Seung-gu Kang,**Jose Antonio Garate**, Xing Tian, Cuicui Ge, Ruhong Zhou "*Protein Corona Mitigates the Cytotoxicity of Graphene Oxide by Reducing Cell Membrane Penetration*" Nanoscale 7;37: 19949-19957 (2015).
- 2015 Hua Yue, Wei Wei, Zonglin Gu, Dezhi Ni,Nana Luo,Zaixing Yang,Lin Zhao, **Jose-Antonio Garate**, Ruhong Zhou, Zhiguo Su and Guanghui Ma "*Exploration of graphene oxide as an intelligent platform for cancer vaccines*" Nanoscale 7;47:19949-19957 (2015).
- 2014 Jiajia Liu, Zaixing Yang, Haotian Li, Zonglin Gu, **Jose-Antonio Garate**, and Ruhong Zhou "*Dewetting transition assisted clearance of (NFGAILS) amyloid fibrils from cell membranes by graphene*" J. Chem. Phys. 14;141:22D520 (2014).
- 2014 **JA Garate**,J Stöckl,María del Carmen Fernández-Alonso,Daniel Artner, Mira Haegman, Chris Oostenbrink, Jesús Jiménez-Barbero, Rudi Beyaert, Holger Heine, Paul Kosma, and Alla Zamyatina "*Anti-endotoxic Activity and Structural basis for human MD-2-TLR4 Antagonism of Tetraacylated Lipid A Mimetics based on  $\beta$ GlcN(1 $\rightarrow$ 1) $\alpha$ GlcN Scaffold*" J. Innate. Immun. doi: 10.1177/1753425914550426 (2014).
- 2014 Raul Araya-Secchi, Tomas Perez-Acle, Seung-gu Kang, Tien Huynh, Alejandro Bernardin, Yerko Escalona, **Jose-Antonio Garate**, Agustin D. Martinez, Isaac E. Garcia, Juan C. Saez, Ruhong Zhou "*Characterization of a Novel Water Pocket Inside the Human Cx26 Hemichannel Structure*" Biophys J. 107 599-612 (2014).
- 2014 **JA Garate**, T Perez-Acle, C Oostenbrink , "*On the thermodynamics of carbon nanotube single-file water loading: free energy, energy and entropy calculations*" Phys. Chem. Chem.Phys. 16, 5119-5128 (2014).
- 2014 B Lai, G Nagy, **JA Garate**, C Oostenbrink , "*Entropic and enthalpic contributions to stereospecific ligand binding from enhanced sampling methods*" J. Chem. Inf. Model. 54 (1) 151-58, (2014).
- 2013 R Reale, NJ English, **JA Garate**, P Marracino, M Liberti, F Apollonio , "*Human aquaporin 4 gating dynamics under and after nanosecond-scale static and alternating electric field impulses: A molecular dynamics study of field effects and relaxation*" J. Chem. Phys 139, 205101 (2013).

- 2013 Artner D, Oblak A, Ittig S, **Garate JA**, Horvat S, Arrieumerlou C, Hofinger A, Oostenbrink C, Jerala R, Kosma P, Zamyatina A. , *Conformationally Constrained Lipid A Mimetics for Exploration of Structural Basis of TLR4/MD-2 Activation by Lipopolysaccharide.* " ACS Chem Biol 8 (11), 2423–32 (2013).
- 2013 **Garate JA**, Oostenbrink C. , *"Free-energy differences between states with different conformational ensembles."* J Comput Chem 34(16),1398-408 (2013).
- 2013 **Garate JA**, Oostenbrink C. , *"Lipid A from lipopolysaccharide recognition: structure, dynamics and cooperativity by molecular dynamics simulations."* Proteins 81(4),658-74 (2013).
- 2012 El-Hendawy MM, **Garate JA**, English NJ, O'Reilly S, Mooney DA, *"Diffusion and interactions of carbon dioxide and oxygen in the vicinity of the active site of Rubisco: molecular dynamics and quantum chemical studies"* J. Chem. Phys 137,145103 (2012).
- 2012 A Singh, R D Gunning, S Ahmed, C A Barrett, N J English, **J-A Garate**, K M Ryan *"Controlled semiconductor nanorod assembly from solution: influence of concentration, charge and solvent nature"* J. Mater. Chem., 22, 1562-69 (2012).
- 2011 **Garate JA**, English NJ, Singh A, Ryan KM, Mooney DA, MacElroy JM, *"Electrophoretic deposition of poly(3-decylthiophene) onto gold-mounted cadmium selenide nanorods."* Langmuir 27(22):13506-13 (2011).
- 2011 R Araya-Secchi, **JA Garate**, DS Holmes, T Perez-Acle, "Molecular Dynamics Study of the Archaeal Aquaporin AqpM Extends the Evidence for a New Family of Aquaporins" BMC Genomics, 12:S8 (2011).
- 2011 **J.-A. Garate**, N.J. English and J.M.D. MacElroy, *"Human aquaporin 4 gating dynamics in dc and ac electric fields: a molecular dynamics study"* J. Chem. Phys 134,055110 (2011).
- 2009 **J.-A. Garate**, N.J. English and J.M.D. MacElroy, *"Static and alternating electric field and distance-dependent effects on carbon nanotube-assisted water self-diffusion across lipid membranes"* J. Chem. Phys 131,114508 (2009).
- 2009 **JA Garate**, M de los Ángeles Valenzuela, MP Gárate, AF Olea *"Aggregation of Alcohols Ethoxylates in n-Heptane"* J Surfact Deterg 12:231–236 (2009).
- 2009 **J.-A. Garate**, N.J. English and J.M.D. MacElroy, *"Carbon nanotube assisted water self-diffusion across lipid membranes in the absence and presence of electric fields"* Molecular Simulation Vol. 35, Nos. 1–2, 3–12 (2009).
- 2008 A. Gonzalez,L. Sepulveda Duran ,R. Araya-Secchi, **J. A. Garate** ,C. D. Pessoa-Mahana,C. F. Lagos,and T. Perez-Acle *"Computational modeling study of functional microdomains in cannabinoid receptor type 1"* Bioorganic and Medicinal Chemistry 16 4378–4389 (2008).
- 2008 M Colombres, **J.A. Garate** ,CF Lagos, R. Araya-Secchi, P. Norambuena, S. Quiroz, L. Larrondo, T. Pérez-Acle, J. Eyzaguirre *"An eleven amino acid residue deletion expands the substrate specificity of acetyl xylan esterase II (AXE II)from Penicillium purpurogenum"*, J Comput Aided Mol Des 22:19–28 (2008).
- \* Corresponding author.

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## Book Chapter

- 2011 N.J. English, **J.-A. Garate** and J.M.D. MacElroy *"Electric-field and friction effects on Carbon nanotube assisted water self-diffusion across lipid membranes"* Carbon Nanotubes - Growth and Applications, InTech, August, 2011.

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## Conferences and Workshops

- July 2014 CINV annual meeting, Valparaiso, Chile.
- September 2013 Biomos meeting, Ausserberg, Switzerland.
- September 2012 Biomos meeting, Ausserberg, Switzerland.
- September 2011 Biomos meeting, Ausserberg, Switzerland.
- July 2011 3DSIG Structural bioinformatics and computational biophysics. Vienna, Austria.
- June 2011 Joint meeting of the Swedish and German Biophysical Societies "Dynamics, function, and design of biological macromolecules Hünfeld, Germany.
- December 2009 ACAM-CECAM Workshop on HPC and Towards Microscale Simulation, Dublin, Ireland
- September 2009 CECAM Summer School on Simulation Approaches to Problems in Molecular and Cellular Biology, San Sebastian, Spain
- July 2009 3<sup>rd</sup> Iberic Meeting on Colloids and Interfaces, Granada Spain.
- November 2008 American Institute of Chemical Engineers Annual Meeting, Philadelphia, USA
- October 2007 Science and Friendship III international meeting, Santiago, Chile
- October 2006 International Conference on Surface and Colloid Science meeting, Beijing, China
- November 2006 29<sup>th</sup> Annual meeting of the Society of Biochemistry and Molecular Biology of Chile, Pucón, Chile.
- November 2006 Structural Bioinformatics Workshop "Molecular Simulations of Transmembrane Proteins: VMD and NAMD", Talca, Chile.
- October 2006 12<sup>th</sup> International Conference on Surface and Colloid Science, Beijing, China.
- July 2006 Postgraduate course in "Structural Bioinformatics", Concepción, Chile.
- October 2004 12<sup>th</sup> Worldwide Congress of Biotechnology, Santiago, Chile.

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## Grants

- 2008-2010 Ad Astra PhD Scholarship, University College Dublin, Dublin, Ireland.
- December 2009 CECAM workshop grant
- September 2009 CECAM workshop grant

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## Academic References

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Oostenbrink,  
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Tomas tomas@dlab.cl  
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