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

September 2017 - present	**Assistant Professor**, *Faculty of Sciences, Universidad de Valparaíso*, Valparaíso, Chile.
September 2017 - present	**Young Research Scientist**, *Millennium Institute Interdisciplinary Center for Neuroscience* , Valparaíso, Chile.
March 2016 - August 2017	**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

2020 - 2022 **ANID Post-Doc project** , *Thermodynamically consistent rule-based models and the circadian clock of Synechococcus elongatus.*

Rol **Sponsor** .

2018 - 2020 **Convocatoria Nacional Subvención a la Instalación en la academia – PAI** , *Inserción de académico con línea de investigación en simulación molecular y nanotoxicidad* .

Rol **Principal Investigator** .

2018 - 2021 **Regular FONDECYT project**, *Molecular mechanisms at the nanobio interphase: applications and biohazards* .

Role **Principal Investigator**.

2018 - 2021 **Regular FONDECYT project**, *Protein insertion in artificial membranes deposited from the vapor phase: From biophysical functionality to nanosensor applications* .

Rol **Co-Investigator**.

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

Role **Investigator**.

2016 - 2019 **Regular 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**.

Teaching

Postgraduate Statistical Mechanics

Postgraduate Computational Biology

Postgraduate Neuronal Excitability

Undergraduate Cellular Physiology

Teaching Experience

November 2017 **International Spring School: Applied Statistical Thermodynamics, from theory to molecular dynamics simulations** , *Fundación Ciencia & Vida.*

Duty Course organizer and Lecturer

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
2014 -2017	**Classical Statistical Thermodynamics**, *Fundación Ciencia & Vida.*
Duty	Course organizer and Lecturer
April 2015 - 2017	**Computational Biology**, *PhD program in Medical Sciences*, Universidad Católica.
Duty	Lecturer
November 2014 - 2017	**Bioinformatics**, *PhD program in Biotechnology*, Universidad Naciónal Andrés Bello.
Duty	Lecturer
2011 - 2013	**Modelling and Simulation of Biomolecules** , *Master program*, Universität für Bodenkultur Wien.
Duty	Lecturer

Peer Reviewed Publications

2020 Mateo Barria-Urenda and **Jose Antonio Garate**, *"Entropy deepens loading chemical potentials of small alcohols by narrow carbon nanotubes"* Phys. Chem. Chem. Phys, 22 (39), 22369-22379 (2020).*

2019 **Jose Antonio Garate**, Alejandro Bernardin, Yerko Escalona, Carlos Yanez, Niall J. English, Tomas Perez-Acle *"Orientational and Folding Thermodynamics via Electric Dipole Moment Restraining"* J. Phys. Chem. B , 123 (12), 2599-2608 (2019).*

2019 Mario Bernardi, Paolo Marracino, Micaela Liberti, **José-Antonio Gárate**, Christian J Burnham, Francesca Apollonio, Niall J English *"Controlling ionic conductivity through transprotein electropores in human aquaporin 4: a non-equilibrium molecular-dynamics study"* Phys. Chem. Chem. Phys., 2019,21, 3339-3346 (2019).

2018 Mario Bernardi, Paolo Marracino, Mohammad Reza Ghaani, Micaela Liberti, Federico Del Signore, Christian J Burnham, **Jose-Antonio Garate**, Francesca Apollonio, Niall J English *"Human aquaporin 4 gating dynamics under axially oriented electric-field impulses: A non-equilibrium molecular-dynamics study"* J. Chem. Phys. 149; 24; 245102 (2018).

2018 Sebastián Contreras-Riquelme, **Jose-Antonio Garate**, Tomas Perez-Acle, Alberto JM Martin *"RIP-MD: a tool to study residue interaction networks in protein molecular dynamics"* Peer. J. 6; e5998 (2018).

2018 Paolo Marracino, Mario Bernardi, Micaela Liberti, Federico Del Signore, Erika Trapani, **Jose-Antonio Garate**, Christian J Burnham, Francesca Apollonio, Niall J English *"Transprotein-Electropore Characterization: A Molecular Dynamics Investigation on Human AQP4"* ACS omega 3 (11), 15361-15369 (2018).

2018 Alessio Borio, Aurora Holgado, **Jose Antonio Garate**, Rudi Beyaert, Holger Heine, Alla Zamyatina *"Disaccharide-Based Anionic Amphiphiles as Potent Inhibitors of Lipopolysaccharide-Induced Inflammation"* Chem. Med. Chem. Phys. Lett, 13;21;2317-2331 (2018).

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_2 surface"* Chem. Phys. Lett, 674; 64-70 (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 βGlcN(1 $\rightarrow$1)αGlcN 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. Garcıa, 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-scalestatic 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.

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.

Academic References

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Tomas Perez-Acle, PhD — tomas@dlab.cl