

ESTEBAN DAVID GADEA

Ph.D. in Chemistry

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CURRENT POSITION

Postgraduate fellow at the Henry Eyring Center for Theoretical Chemistry at The University of Utah under the supervision of Valeria Molinero.

AREAS OF EXPERTISE

Computational simulation of chemical systems across multiple scales, within the fields of electrochemistry, phase transitions, and light-matter interactions.

EDUCATION

- 4/2018 - 8/2023 **Ph.D. in Inorganic Chemistry, Analytical Chemistry and Physical Chemistry** Universidad de Buenos Aires
Under the supervision of Prof. Damian Scherlis, studying electronic dynamics in electrochemical interfaces and nucleation of bubbles on electrodes.
- 2/2012 - 3/2018 **Chemistry degree** Universidad Nacional de La Plata
Undergraduate degree in chemistry (equivalent to a MSc. in Chemistry) at age 24 (GPA 3.7)

PUBLICATIONS

- 2025 **Nanoparticle Electrodes Trigger Bubble Detachment and Enhance Gas Evolution Efficiency** ACS nano
KWang, ED Gadea, BR Money, YA Perez Sirkin, DA Scherlis, HS White, V Molinero
- 2025 **Ether Cleavage Decreases the Ion Exchange Capacity of Anion Exchange Membranes** Chem. Mater.
S Erimban, MH Factorovich, IJ Bombau, JJ Karnes, ED Gadea, JJ Schwartz, V Molinero
- 2024 **Interplay between classical and quantum dissipation in light-matter dynamics** JCP
F Tarasi, TN Todorov, CM Bustamante, ED Gadea, L Stella, T Apostolov, DA Scherlis
- 2024 **The smallest electrochemical bubbles** PNAS
ED Gadea, YA Perez Sirkin, V Molinero, DA Scherlis
- 2024 **Modeling the electroluminescence of atomic wires from quantum dynamics simulations** JCP
CM Bustamante, T Todorov, ED Gadea, F Tarasi, L Stella, A Horsfield, DA Scherlis
- 2023 **Nanobubble Stability and Formation on Solid-Liquid Interfaces in Open Environments** Nano Lett.
ED Gadea, V Molinero, DA Scherlis
- 2023 **Fluorescence in quantum dynamics: Accurate spectra require post-mean-field approaches** JCP
CM Bustamante, ED Gadea, TN Todorov, A Horsfield, L Stella, DA Scherlis
- 2022 **Tailoring Cooperative Emission in Molecules: Superradiance and Subradiance from First-Principles Simulations** JPC Lett.
CM Bustamante, ED Gadea, TN Todorov, DA Scherlis
- 2022 **Radiative thermalization in semiclassical simulations of light-matter interaction** PRA
ED Gadea, CM Bustamante, TN Todorov, DA Scherlis
- 2021 **Dissipative equation of motion for electromagnetic radiation in quantum dynamics** PRL
CM Bustamante, ED Gadea, A Horsfield, TN Todorov, MC González Lebrero, DA Scherlis
- 2020 **Electrochemically Generated Nanobubbles: Invariance of the Current with Respect to Electrode Size and Potential** JPC Lett.
ED Gadea, YA Perez Sirkin, V Molinero, DA Scherlis
- 2019 **Mechanisms of nucleation and stationary states of electrochemically generated nanobubbles** JACS
YA Perez Sirkin, ED Gadea, DA Scherlis, V Molinero

SCIENTIFIC VISITS

During the Ph.D. program

- 8/2023 - 11/2023 **School of Mathematics and Physics Queen's University Belfast** United Kingdom
Three month secondment as part of the European project ATLANTIC studying exciton dynamics
- 5/2023 - 6/2023 **International Centre for Theoretical Physics** Italy
As part of the Simons Associates program
- 7/2022 - 9/2022 **Henry Eyring Center for Theoretical Chemistry at The University of Utah** USA
Three month internship at the Molinero Group studying thermodynamic stability of bubbles in open environments

1/2020 - 3/2020	School of Mathematics and Physics Queen's University Belfast Three month secondment as part of the European project ATLANTIC studying radiative thermalization	United Kingdom
7/2019 - 9/2019	Henry Eyring Center for Theoretical Chemistry at The University of Utah Eight weeks internship at the Molinero Group studying electrochemically generated nanobubbles	USA

CONFERENCES

2025	Electronic Materials and Applications Composition-Driven Electrocatalysis: High-Entropy Perovskites for Oxygen Evolution Reaction	USA
2024	Molecular Interactions and Dynamics Gordon Research Conference Electrocatalytic Landscapes: Understanding Interaction Effects in High-Entropy Perovskite Oxides as OER catalysts	USA
2023	Workshop on Frontiers in Excited State Electronic Structure Methods: from Spectroscopy to Photochemistry Radiative thermalization in semiclassical simulations of light-matter interaction	Italy
2023	XXIII Congreso Argentino de Fisicoquímica y Química Inorgánica Producción electroquímica de gas controlada por la formación de nanoburbujas	Argentina
2022	I Simposio de Modelado Multiescala para Biociencias y Nanomateriales Producción electroquímica de gas controlada por la formación de nanoburbujas	Argentina (online)
2022	American Conference on Theoretical Chemistry Electrochemically Generated Nanobubbles: Invariance of the Current with Respect to Electrode Size and Potential	USA
2021	XXII Congreso Argentino de Fisicoquímica y Química Inorgánica Nanoburbujas generadas electroquímicamente: modelado y simulación de la respuesta corriente potencial	Argentina (online)
2020	ICTP On-line Workshop on Excited Charge Dynamics in Semiconductors Radiative Decay in Real-Time Electron Dynamics	Italy (online)
2019	Chemistry and Physics of Liquids Gordon Research Conference and Seminar Molecular Modeling of the Nucleation of Electrochemically Generated Nanobubbles	USA
2019	ICTP Caribbean School on Materials for Clean Energy Modeling Electrochemically Generated Nanobubbles	Colombia
2019	XXI Congreso Argentino de Fisicoquímica y Química Inorgánica Modelado de burbujas de escala nanométrica generadas electroquímicamente	Argentina
2017	XX Congreso Argentino de Fisicoquímica y Química Inorgánica Estudio computacional de la inhibición de N- β -glicosilsulfamidas y S- β -glicosilsulfonamidas análogos sobre la anhidrasa carbónicas	Argentina

TEACHING EXPERIENCE

3/2018 - 8/2023	Teaching Assistant Analytical Chemistry and Instrumental Chemistry	Universidad Nacional de La Plata
6/2015 - 3/2018	Undergraduate Teaching Assistant Analytical Chemistry and Instrumental Chemistry	Universidad Nacional de La Plata

AWARDS

2023 Best Poster in Computational and Theoretical Chemistry
Awarded by XXIII Congreso Argentino de Fisicoquímica y Química Inorgánica

2022 Best Poster
Awarded by I Simposio de Modelado Multiescala para Biociencias y Nanomateriales

LANGUAGES

English - advanced, **Spanish** - native

SKILLS

Programming languages: Fortran, C, C++, Python, Julia.

Softwares: Lammmps, Amber, NAMD, AutoDock, AutoDock Vina, Gaussian, Orca, Quantum Espresso, Comsol, Zacros, VMD, Ovito.

Techniques: Molecular dynamics, Monte Carlo, kinetic Monte Carlo, density functional theory, time-dependent density functional theory, tight-binding.

REFERENCES

Damian A. Scherlis Associate professor at Universidad de Buenos Aires - damian@qi.fcen.uba.ar.

Valeria Molinero Distinguished professor at the University of Utah - valeria.molinero@utah.edu.

Tchavdar N. Todorov Reader at Queen's University Belfast - t.todorov@qub.ac.uk.