ESTEBAN DAVID GADEA

Ph.D. in Chemistry

Salt Lake City, Utah, United States of America

esteban.gadea@utah.edu

github.com/estebangadea

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, Analitical 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** — **United Kingdom**
Three month secondment as part of the European project ATLANTIC studying radiative thermalization

7/2019 - 9/2019 **Henry Eyring Center for Theoretical Chemistry at The University of Utah** — **USA**
Eight weeks internship at the Molinero Group studying electrochemically generated nanobubbles

CONFERENCES

2025 **Electronic Materials and Applications** — **USA**
Composition-Driven Electrocatalysis: High-Entropy Perovskites for Oxygen Evolution Reaction

2024 **Molecular Interactions and Dynamics Gordon Research Conference** — **USA**
Electrocatalytic Landscapes: Understanding Interaction Effects in High-Entropy Perovskite Oxides as OER caralysts

2023 **Workshop on Frontiers in Excited State Electronic Structure Methods: from Spectroscopy to Photochemistry** — **Italy**
Radiative termalization in semiclassical simulations of light-matter interaction

2023 **XXIII Congreso Argentino de Fisicoquímica y Química Inorgánica** — **Argentina**
Producción electroquímica de gas controlada por la formación de nanoburbujas

2022 **I Simposio de Modelado Multiescala para Biociencias y Nanomateriales** — **Argentina (online)**
Producción electroquímica de gas controlada por la formación de nanoburbujas

2022 **American Conference on Theoretical Chemistry** — **USA**
Electrochemically Generated Nanobubbles: Invariance of the Current with Respect to Electrode Size and Potential

2021 **XXII Congreso Argentino de Fisicoquímica y Química Inorgánica** — **Argentina (online)**
Nanoburbujas generadas electroquímicamente: modelado y simulación de la respuesta corriente potencial

2020 **ICTP On-line Workshop on Excited Charge Dynamics in Semiconductors** — **Italy (online)**
Radiative Decay in Real-Time Electron Dynamics

2019 **Chemistry and Physics of Liquids Gordon Research Conference and Seminar** — **USA**
Molecular Modeling of the Nucleation of Electrochemically Generated Nanobubbles

2019 **ICTP Caribbean School on Materials for Clean Energy** — **Colombia**
Modeling Electrochemically Generated Nanobubbles

2019 **XXI Congreso Argentino de Fisicoquímica y Química Inorgánica** — **Argentina**
Modelado de burbujas de escala nanométrica generadas electroquímicamente

2017 **XX Congreso Argentino de Fisicoquímica y Química Inorgánica** — **Argentina**
Estudio computacional de la inhibición de N-β-glicosilsulfamidas y S-β-glicosilsulfonamidas análogas sobre la anhidrasa carbónicas

TEACHING EXPERIENCE

3/2018 - 8/2023 **Teaching Assistant** — **Universidad Nacional de La Plata**
Analytical Chemistry and Instrumental Chemistry

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

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: Lammps, 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.