

# William R. Borrelli

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## SUMMARY

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Computational scientist with expertise at the intersection of atomistic simulation, data science/machine-learning, and statistical mechanics and thermodynamics. Seeking industry roles that involve quantitatively rigorous decision-making and creating actionable data-driven insights.

## PROFESSIONAL EXPERIENCE

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**Graduate Researcher - Department of Chemistry & Biochemistry** May 2022 – Present  
*University of California, Los Angeles* Los Angeles, CA

- Devised and executed computational research on the solution phase chemistry of hydrated electrons and alkali dimers
- Managed and collaborated on the research projects of undergraduate students, junior graduate students, and an experimentally trained postdoctoral researcher
- Published numerous peer-reviewed publications in prestigious chemistry and chemical physics journals

**Computational Materials Science Intern** June 2025 – August 2025  
*Corporate Research in Materials Engineering at Robert Bosch LLC* Watertown, MA

- Developed and bench-marked a computational workflow for calculating thermodynamic measures of solution non-ideality for corrosion modeling
- Collaborated with an interdisciplinary and international team of materials scientists, engineers, and physicists to guide industry research and development goals

**ACCESS Allocation Manager** September 2024 - Present  
*University of California, Los Angeles* Los Angeles, CA

- Wrote peer-reviewed proposals resulting in grants of over 1 million high-performance computing CPU hours for computational chemical physics research

**Undergraduate Researcher** October 2019 – July 2021  
*Fordham University* The Bronx, NY

- Wrote Python code for automated sampling of high-dimensional chemical space constrained by attainable reaction conditions

## EDUCATION

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**University of California, Los Angeles** Los Angeles, CA  
*PhD in Theoretical & Computational Chemistry* September 2021 – 2026 (Expected)

**Fordham University (Magna Cum Laude)** The Bronx, NY  
*B.S. in Chemistry, minor in Psychology* August 2017 – May 2021

## SELECTED PUBLICATIONS

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(Find the rest on my [website](#))

- Roles of H-Bonding and Hydride Solvation in the Reaction of Hydrated (Di)electrons with Water to Create H<sub>2</sub> and OH<sup>-</sup> (J. Chem. Theory Comput. 2024, 20, 16, 7337–7346)
- Using Machine Learning to Understand the Causes of Quantum Decoherence in Solution-Phase Bond Breaking Reactions (J. Phys. Chem. Lett. 2024, 15, 4, 903–911)

## PRESENTATIONS & OTHER PROFESSIONAL INVOLVEMENT

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**SoCal Theochem 2023 - Talk** October 14, 2023  
*University of California, Los Angeles* Los Angeles, CA

- Title: Solvation Entropy Calculations for Different Models of the Hydrated Electron

**UCLA Chemistry & Biochemistry Graduate Admissions Student Reviewer** December 2024  
*University of California, Los Angeles* Los Angeles, CA

- Collaborated with faculty members in evaluating PhD student applications for the Theory and Computation Specialization at UCLA

**Co-organizer of SoCal Theochem 6 Conference** October 2023  
*University of California, Los Angeles* Los Angeles, CA

- Built and maintained the conference website coded in HTML - allowed for hyperlink registration and an embedded map of UCLA and the surrounding area