Yair Ezequiel Litman

Date and Place of Birth:	16 October 1990, Buenos Aires, Argentina
Nationality:	Argentinean and Polish
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Online profiles:	LinkedIn, Google Scholar, Orcid,

Education

2016-2020 | **Dr. rer. nat.** (Grade: *summa cum laude*)
Fritz Haber Institute of the Max Planck Society and Freie Universität Berlin

2009-2014 | **Licenciate in Chemical Sciences**
University of Buenos Aires, MSc. degree equivalent
(GPA: 9.27/10)

Research Experience

Mar 2026 – Present | **Junior Faculty**
Max Planck Graduate Center mit der Johannes Gutenberg-Universität (MPGC)

Apr 2025 – Present | **Group Leader**
Max Planck Institute for Polymer Research
Department of Molecular Spectroscopy (Director: Prof. Mischa Bonn)

Mar 2022 – Mar 2025 | **Research Associate (Walter Benjamin Fellow)**
Yusuf Hamied Department of Chemistry, University of Cambridge
Supervisors: Stuart Althorpe and Angelos Michaelides

Sep 2021 – Feb 2022 | **Postdoctoral Position**
Max Planck Institute for Polymer Research (MPIP)
Supervisors: Yuki Nagata and Mischa Bonn

Aug 2020 – Aug 2021 | **Postdoctoral Position**
Max Planck Institute for the Structure and Dynamics of Matter (MPSD)
Supervisor: Mariana Rossi

Oct 2016 – Aug 2020 | **Doctoral Studies**
PhD student at the Fritz Haber Institute of The Max Planck Society (FHI)
Thesis title: Tunneling and Zero-Point Energy Effects in Multidimensional Hydrogen Transfer Reactions: From Gas Phase to Adsorption on Metal Surfaces. Supervisor: Mariana Rossi. Co-supervisor: Beate Paulus (Freie Universität)

Funding & Awards

- Max Planck BAR funding to install a GPU cluster at Max Planck Computing and Data Facility (**536.000 EUR**, 2025)
- Rückkehrprogramm, Ministry of Culture and Science, North Rhine-Westphalia, Germany. (**1.25 Mill. EUR**, 2024)
- Junior Research Fellowship. Wolfson College, University of Cambridge (**2400 GBP**, 2023)
- Poster Prize. Vibrational Spectroscopy GRC. Rhode Island, United States (2022)

- Selected to attend the 70th Lindau Nobel Laureate Meeting (2022)
- DAAD Travel Fellowship (**2000 EUR**, 2022)
- Walter Benjamin Fellowship, German Research Foundation (DFG) (**84000 EUR**, 2021)
- Newton International Fellowship, Royal Society (**105000 GBP**, 2021)
- Poster Prize, 81st Okazaki Conference, Okazaki, Japan (2019)
- Poster Prize. CECAM/Psi-k school on "Path Integral Quantum Mechanics" (2018)
- DAAD Travel Fellowship (**2000 EUR**, 2018)
- Computational resources at the CSCS National Supercomputing Centre (16 million core hours, 2018)
- Medal of Honor: 3rd highest GPA (Chemistry, University of Buenos Aires, 2015)

Other Professional activities

Reviewing Activities

Reviewer of 40+ scientific manuscripts: The Journal of Chemical Physics (16), The Journal of Physical Chemistry (9), Journal of the American Chemical Society (3), Journal of Chemical Theory and Computation (3), Angewandte Chemie (2), Nature Communications (3), The Journal of Physical Chemistry Letters (2), Journal of Molecular Liquids (2), and ACS Nano (1).

Supervision & Mentoring

- Supervision of one PhD student and two postdocs (Max Planck Institute for Polymer Research, Present)
- Co-supervision of one master's thesis project (University of Cambridge, 2023) (The student received the award for best theoretical thesis of the year)
- Co-supervision of several projects involving three PhD students (University of Cambridge, 2022-2024)
- Co-supervision of one project involving one PhD student (MPSD, Germany, 2023-2024)

Teaching

- Teaching Assistant. (University of Cambridge, 2022)
- Teaching Assistant. (University of Buenos Aires, 2015-2016)
- Tutor for Practical Exercises (CECAM Flagship School on Path Integrals, Tel Aviv, 2023)
- Tutor for Practical Exercises (Hands-On DFT and Beyond Workshop, Berlin 2017 and Barcelona, 2019)

Organizer of Scientific Events

- CECAM Flagship School. SpectroDynamics 2026: Connecting Computational Spectroscopic Methods Across the Electromagnetic Spectrum. Event website
  60 participants, 5-day program, CECAM-HQ-EPFL, Lausanne, Switzerland, 2026
- CECAM Flagship Workshop. The Atomic Simulation Environment: Integration into Wider Community Projects. Event website
  60 participants, 5-day program, CECAM-DE-SMSM Mainz, Germany, 2026
- 3rd n-Aqua Workshop.
  58 participants, 3.5-day program, Kalamata, Greece, 2024
- CECAM Flagship School. Path Integral Quantum Mechanics. Event website
  68 participants, 5-day program, Tel-Aviv University, Tel-Aviv, Israel, 2023
- CECAM Flagship School. Path Integral Quantum Mechanics: From the Basics to the Latest Developments. Event website
  112 participants, 5-day program, virtual event, 2021

Contributions to Scientific Open-Source Software

- Main co-developer of the i-PI code.
- Regular contributor to the FHI-aims code.

Contributions to Equality, Diversity, and Inclusion (EDI) in Academia

- Organizer of Lennard-Jones Centre Gender Equality Network panel discussion (2025)
- Organizer of EDI activities at the Molecular Spectroscopy Department retreat (2025)
- Organizer of the inaugural kick-off meeting of the Lennard-Jones Centre Gender Equality Network (2024)
- reator and maintainer of an EDI resources repository.

Workshops, Meetings and Conferences

Invited Talks

May 2026	**Deciphering the Structure and Reactivity of Water at Interfaces and under Confinement using MLIPs** 4th SIMPLAIX Workshop on Machine Learning for Multiscale Molecular Modeling, Heidelberg, Germany.
Apr 2026	**Unraveling Water's Behavior in Anisotropic Environments** SFB TACO, Vienna University of Technology and University of Vienna, Vienna, Austria.
Apr 2026	**Molecular Strategies for Confinement-Controlled Water Structure and Chemistry** Department of Chemistry, Fudan University, Shanghai, China
Apr 2026	**Unraveling Water's Behavior in Anisotropic Environments** Basic Research Center of Excellence for Quantum Science, Southern University of Science and Technology (SUSTEC), Shenzhen, China
Apr 2026	**Two Tales of Water under Electric Fields: When Entropy Matters and Interfaces Mislead** International Conference on Chemical Reactivity in Droplets and at Air-Water Interfaces, Shanghai, China
Mar 2026	**Unraveling Water's Behavior in Anisotropic Environments** INQUIMAE, University of Buenos Aires, Buenos Aires, Argentina
Nov 2025	**Introduction to ab initio Molecular Dynamics** Hands-On Workshop on Electronic Structure Theory and Artificial Intelligence for Material Science, Shanghai University, Shanghai, China
Sep 2025	**Molecular Strategies for Confinement-Controlled Water Structure and Chemistry** 3rd International Symposium on Confinement-Controlled Chemistry, Ruhr University Bochum, Bochum, Germany
Jul 2025	**Surprises in the Structure and Reactivity of Water under Large Electric Fields** CECAM Workshop: Simulations of Electrochemical Storage Devices: from Quantum to Classical Descriptions, Sorbonne University, Paris, France
May 2025	**Spectroscopy Crash Course** Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge, United Kingdom
May 2025	**Entropy Governs the Structure and Reactivity of Water Dissociation under Electric Fields** CECAM Workshop: Chemical Reactivity in Aerosols and at Air-Water Interfaces, Ecole Normale Supérieure, Paris, France
Feb 2025	**Unraveling the Behavior of Water in Anisotropic Environments** Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge, United Kingdom
May 2024	**First-Principles Simulations of Tip-Enhanced Raman Spectroscopy** FHI-aims UK Meeting, University of Warwick, United Kingdom

Feb 2024 | **Decoding Aqueous Interfaces with Molecular Dynamics Simulations and Surface-Specific Spectroscopies**
Department of Chemistry, Tel Aviv University, Tel Aviv, Israel

Feb 2024 | **Surface-Specific Spectroscopy from First Principles**
Department of Chemistry, Ben Gurion University, Beersheba, Israel

Sep 2023 | **New Insights on Aqueous Electrolyte Interfaces** (Selected poster presentation)
The Inaugural Lennard-Jones Centre Meeting, Cambridge, United Kingdom

Aug 2023 | **Simulation of Tip-Enhanced Raman Spectroscopy**
FHI-aims Users' and Developers' Meeting, Hamburg, Germany

Jun 2023 | **Tunneling and Zero-Point Energy Effects in Multidimensional Hydrogen Transfer Reactions**
Department of Biological Physics and Molecular Chemistry and Department of Materials Science, Weizmann Institute, Rehovot, Israel

Jun 2023 | **Surface-specific Spectroscopy from First Principles**
Schulich Faculty of Chemistry, Technion University, Haifa, Israel

Jul 2022 | **Surface-Sensitive Spectroscopy with Ab Initio Accuracy Using Machine Learning**
Vibrational Spectroscopy, Gordon Research Seminar, Rhode Island, United States

Jul 2022 | **Let the Atoms dance with i-PI**
Summer School on Theoretical Modelling at the Nanoscale, Ringberg, Germany

Jun 2022 | **Tunneling and Zero-Point Energy Effects in Multidimensional Hydrogen Transfer Reactions**
Lennard-Jones Centre, Cambridge, United Kingdom

Apr 2021 | **Tunneling and Zero-Point Energy Effects in Multidimensional Hydrogen Transfer Reactions**
Computational Surface Science Group Seminar (Prof. Maurer), University of Warwick, United Kingdom

Nov 2018 | **Elucidation of the Quantum Dynamics of Intramolecular Proton Transfer Reaction in Porphycene**
Workshop on H-bonding/transfer dynamics of porphycene and its derivatives, Warsaw, Poland

Contributed Talks (since 2019)

Dec 2025 | **Surprises in the Structure and Reactivity of Water under Large Electric Fields**
Y. Litman, A. Michaelides
Lorentz Workshop: Interfacial H_2O: Shaping the Electric Double Layer, Leiden, Netherlands

Aug 2025 | **Entropy Governs the Structure and Reactivity of Water Dissociation under Electric Fields**
Y. Litman, A. Michaelides
Psi-k, Lausanne, Switzerland

Mar 2025 | **Field-Induced Water Autoionization in Two- and Three-dimensions**
Y. Litman, A. Michaelides
DPG (Deutsche Physikalische Gesellschaft) Spring Meeting. Regensburg, Germany.

Mar 2024 | **Surface Stratification Determines the Interfacial Water Structure of Simple Electrolyte Solutions**
Y. Litman, K-Y. Chiang, T. Seki, Y. Nagata, M. Bonn.
DPG (Deutsche Physikalische Gesellschaft) Spring Meeting. Berlin, Germany.

Mar 2023 | **Surface-Sensitive Spectroscopy from First Principles**
Y. Litman, J. Lan, K-Y. Chiang, V. Kapil, Y. Nagata, D. Wilkins.
DPG (Deutsche Physikalische Gesellschaft) Spring Meeting. Dresden, Germany.

Sep 2022 | **The Surface of Electrolyte Solutions is Stratified**
Y. Litman, K-Y. Chiang, T. Seki, Y. Nagata, M. Bonn
DPG (Deutsche Physikalische Gesellschaft) Spring Meeting. Regensburg, Germany.

Sep 2022 | **Incorporating First-Principles Electronic Friction in Instanton Rate Theory**
Y. Litman, E. S. Pos, C. L. Box, R. Martinazzo, R. J. Maurer, M. Rossi
DPG (Deutsche Physikalische Gesellschaft) Spring Meeting. Regensburg, Germany.

Sep 2021 | **Surface Vibrations Enhance Intramolecular Hydrogen Tunneling in (some) Molecular Switches**
Y. Litman, M. Rossi
APS (American Physical Society) March Meeting. Online event.

Sep 2019 | **Temperature Dependence of the Vibrational Spectrum of Porphycene**
Y. Litman, J. Behler, M. Rossi
Faraday Discussion: Quantum effects in complex systems. Coventry, United Kingdom.

Apr 2019 | **Elucidation of the Quantum Dynamics of Intramolecular Proton Transfer Reaction in Porphycene**
Y. Litman, T. Kumagai, J. O. Richardson, M. Rossi
DPG (Deutsche Physikalische Gesellschaft) Spring Meeting. Regensburg, Germany.

Mar 2019 | **Elucidation of the Quantum Dynamics of Intramolecular Proton Transfer Reaction in Porphycene**
Y. Litman, T. Kumagai, J. Richardson, M. Rossi
APS (American Physical Society) March Meeting. Boston, USA.

Feb 2019 | **Elucidation of the Quantum Dynamics of Intramolecular Proton Transfer Reaction in Porphycene**
Y. Litman, T. Kumagai, J. Richardson, M. Rossi
Workshop on Theoretical Chemistry 2019 Path Integral Methods for Nuclear Quantum Effects. Mariapfarr, Austria.

Yair Litman – Publikationsliste (April 2026)

(* = Korrespondierender Autor, ‡ = Gleiche Mitwirkung)

1. **Wetting Transparency of Graphene: A macroscopic Window but Nanoscopic Mirror**
   Accepted in Chem, arXiv:2511.04930 2025
   Wang, Y‡*; Litman, Y‡*; Cho, M; Cox, S; Bonn, M*.

2. **Breaking the Air–Water Paradigm: Ion Behavior at Hydrophobic Solid–Water Interfaces**
   Journal of the American Chemical Society, *2026, 148, 12753*
   Advincula, X. R; Fong, K. F; Wang, Y; Schran, C; Bonn, M; Michaelides, A*; Litman, Y*

3. **Infrared and Raman Perspectives on Vibrational Coupling in Liquid Water**
   Accepted in Journal of Chemical Physics
   Haggard, C; Litman, Y*; Althorpe, S.

4. **Tip-Enhanced Raman Images of Realistic Systems through Ab Initio Modeling**
   ACS Nano, *2026, 20, 5550*
   Brezina, K*; Litman, Y; Rossi, M*.

5. **Entropy Governs the Structure and Reactivity of Water Dissociation under Electric Fields** (Selected as Cover Image)
   Journal of the American Chemical Society, *2025, 147, 44885*
   Litman, Y*; Michaelides, A*.

6. **How reactive is water at the nanoscale and how to control it?**
   arXiv:2508.13034 2025
   Advincula, X.R; Litman, Y; Fong, K. D; Witt, W. C; Schran, C*; Michaelides, A*.

7. **Reevaluating Anomalous Electric Fields at the Air-Water Interface: A Surface-Specific Spectroscopic Survey**
   Journal of the American Chemical Society, *2025, 147, 46163*
   Shirley, J. C; Xuan Ng, Z; Chiang, K-Y; Nagata, Y; Litman, Y; Hazrah, A. S*; Bonn, M*.

8. **Roadmap on advancements of the FHI-aims software package**
   arXiv:2505.00125 2025
   (100+ authors)

9. **Surface Stratification Determines the Interfacial Water Structure of Simple Electrolyte Solutions**
   Nature Chemistry, *2024, 16, 644*
   Litman, Y*‡; Chiang, K‡; Seki, T; Nagata, Y; Bonn, M*.

10. **Quantum Rates in Dissipative System with Spatially Variable Friction**
    The Journal of Chemical Physics, *2024, 161, 024110*
    Bridge, O; Martinazzo, R; Rossi, M; Althorpe, S; Lazzaroni, P; Litman, Y*.

11. **i-PI 3.0: a flexible and efficient framework for advanced atomistic simulations**
    The Journal of Chemical Physics, *2024, 161, 062504*
    Litman, Y; Kapil, V; Feldman, Y; Tisi, D; Begusic, T; Fidanyan, K; Fraux, G; Higer, J; Kellner, M; Li, T. E; Pós, E. S; Stocco, E; Trenins, G; Hirshberg, B; Rossi, M*; Ceriotti, M.*

12. **Thermal quenching of classical and semiclassical scrambling**
    Physical Review E, *2024, 110, L012204*
    Sadhasivam, V. G; Hunt, A. C; Meuser, L; Litman, Y; Althorpe, S. C.*

13. **Learning Electronic Polarizations in Aqueous Systems**
    Journal of Chemical Information and Modeling, *2024, 64, 4426*
    Jana, A; Shepherd, S; Litman, Y; Wilkins, D. M*.

14. **Fully First-Principles Surface Spectroscopy with Machine Learning**
The Journal of Physical Chemistry Letters, *2023, 14, 8175*
Litman, Y*; Lan, J; Nagata, Y; Wilkins, D. M*.

15. **First-Principles Simulations of Tip-enhanced Raman Scattering Imaging Reveal Atomic Scale Chemical Enhancement**
The Journal of Physical Chemistry Letters, *2023, 14, 6850*
Litman, Y*‡; Bonafe, F‡; Akkoush, A; Appel, H; Rossi, M*.

16. **A Hybrid-DFT Study of Intrinsic Point Defects in MX2 (M=Mo, W; X=S, Se) Monolayers**
Physica Status Solidi A: Applications and Materials Science, *2023, 2300180*
Akkoush, A*; Litman, Y; Rossi, M.*

17. **Is Unified Understanding of Vibrational Coupling of Water Possible? Hyper-Raman Measurements and Machine Learning Spectra**
The Journal of Physical Chemistry Letters, *2023, 14, 3063*
Inoue, K‡; Litman, Y‡; Wilkins, D. M.; Nagata, Y*; Okuno, M*.

18. **Dissipative Tunneling Rates through the Incorporation of First-Principles Electronic Friction in Instanton Rate Theory II: Benchmarks and Applications**
The Journal of Chemical Physics, *2022, 156, 194107*
Litman, Y*; Pós, E. S; Connor, L. B; Martinazzo, R; Maurer, R. J; Rossi, M*.

19. **Dissipative Tunneling Rates through the Incorporation of First-Principles Electronic Friction in Instanton Rate Theory I: Theory**
The Journal of Chemical Physics, *2022, 156, 194106*
Litman, Y*; Pós, E. S; Connor, L. B; Martinazzo, R; Maurer, R. J; Rossi, M*.

20. **Charge Transfer Mediated Dramatic Enhancement of Raman Scattering upon Molecular Point Contact Formation**
Nano Letters, *2022, 22, 2170–2176*
Cirera, B; Litman, Y; Chenfang, L; Akkoush, A; Hammud, A; Wolf, M; Rossi, M; Kumagai, T*.

21. **Multidimensional Hydrogen Tunneling in Supported Molecular Switches: The Role of Surface Interactions**
Physical Review Letters, *2020, 125, 216001*
Litman, Y*; Rossi, M*.

22. **Temperature Dependence of the Vibrational Spectrum of Porphycene: A Qualitative Failure of Classical-Nuclei Molecular Dynamics**
Faraday Discussions, *2020, 221, 526-546*.
Litman, Y; Behler, J; Rossi, M*.

23. **Zero-point energy and tunnelling: general discussion**
Faraday Discussions, *2020, 221, 478-500*
(*Authors given in alphabetic order*)
Althorpe, S; Alvertis, A; Barford, W; Benson, R; Burghardt, I; Giannini, S; Habershon, S; Hammes-Schiffer, S; Hay, S; Iyengar, S; Kelly, A; Komarova, K; Lawrence, J; Litman, Y; Martens, C; Maurer, R; Plant, D; Rossi, M; Sakaushi, K; Schile, A; Sturniolo, S; Tew, D; Trenins, G; Worth, G.

24. **Emerging opportunities and future directions: general discussion**
Faraday Discussions, *2020, 221, 564-581* (*Authors given in alphabetic order*)
Althorpe, S; Barford, W; Blumberger, J; Bungey, C; Burghardt, I; Datta, A; Ghosh, S; Giannini, S; Grünbaum, T; Habershon, S; Hammes-Schiffer, S; Hay, S; Iyengar, S; Jones, G; Kelly, A; Komarova, K; Lawrence, J; Litman, Y; Mannouch, J; Manolopoulos, D; Martens, C; Maurer, R; Melander, M; Rossi, M; Sakaushi, K; Saller, M; Schile, A; Sturniolo, S; Tre-

nins, G; Worth, G.

25. **Spectroscopic signatures of quantum effects: general discussion**
Faraday Discussions, *2020, 221, 322-349* (*Authors given in alphabetic order*)
Alvertis, A; Barford, W; Bourne Worster, S; Burghardt, I; Chin, A; Datta, A; Dijkstra, A; Fay, T; Fielding, H; Grünbaum, T; Habershon, S; Hammes-Schiffer, S; Iyengar, S; Jones, A; Komarova, K; Léonard, J; Litman, Y; Picconi, D; Plant, D; Schile, A; Scholes, G; Segarra-Martí, J; Segatta, F; and Troisi, A; Worth, G.

26. **Quantum coherence in complex environments: general discussion**
Faraday Discussions, *2020, 221, 168-201* (*Authors given in alphabetic order*)
Alvertis, A; Barford, W; Bourne Worster, S; Burghardt, I; Datta, A; Dijkstra, A; Fay, T; Ghosh, S; Grünbaum, T; Habershon, S; Hore, P; Hutchinson, D; Iyengar, S; Jones, A; Jones, G; Komarova, K; Lawrence, J; Léonard, J; Litman, Y; Mannouch, J; Manolopoulos, D; Martens, C; Mondelo-Martell, M; Picconi, D; Plant, D; Sakaushi, K; Saller, M; Schile, A; Scholes, G; Segarra-Martí, J; Segatta, F; Troisi, A; Worth, G.

27. **Elucidating the Nuclear Quantum Dynamics of Intramolecular Double Hydrogen Transfer in Porphycene**
Journal of the American Chemical Society, *2019, 141, 2526-2534* (Selected as Cover Image).
Litman, Y; Richardson, J; Kumagai, T; Rossi, M*.

28. **i-PI 2.0: A Universal Force Engine for Advanced Molecular Simulations**
Computer Physics Communications, *2019, 236, 214-223*
Kapil, V; Rossi, M; Marsalek, O; Petraglia, R; Litman, Y; Spura, T; Bingqing, C; Cuzzocrea, A; Meißner, R; Wilkins, D; Helfrecht, B; Przemyslaw, J; Bienvenue, S; Fang, W; Kessler, J; Poltavsky, I; Vandenbrande, S; Wieme, J; Corminboeuf, C; Kühne, T; Manolopoulos, D; Markland, T; Richardson, J; Tkatchenko, A; Tribello, G; Van Speybroeck, V; Ceriotti, M*.

29. **Decisive Role of Nuclear Quantum Effects on Surface Mediated Water Dissociation at Finite Temperature**
The Journal of Chemical Physics, *2018, 148, 102320*
Litman, Y; Donadio, D; Ceriotti, M; Rossi, M*.

30. **Photophysics of Xanthene Dyes at High Concentrations in Solid Environments: Charge Transfer Assisted Triplet Formation**
Photochemistry and Photobiology, *2018, 94, 865-874*
Litman, Y; Rodríguez, H; Braslavsky, S; San Román, E*.

31. **Quantum Tunneling in Real Space: Tautomerization of Single Porphycene molecules on the (111) surface of Cu, Ag, and Au**
The Journal of Chemical Physics, *2018, 148, 102330*
Kumagai, T*; Ladenthin, J; Litman, Y; Rossi, M*; Grill, L; Gawinkowski, S; Waluk, J; Persson, M.

32. **Positional Isotope Exchange in $HX\cdots(H_2O)_n (X = F, I)$ Clusters at Low Temperatures**
The Journal of Physical Chemistry A, *2016, 120, 7213-7224*
Litman, Y; Videla, P; Rodriguez, J; Laria, D*.

33. **Tuning the Concentration of Dye Loaded Polymer Films for Maximum Photosensitization Efficiency: Phloxine B in Poly(2-hydroxyethyl methacrylate)**
Photochemistry and Photobiology Sciences, 2016, 15, 80-85
Litman, Y; Rodríguez, H; San Román, E*.

34. **Effect of concentration on the Rose Bengal triplet state formation on microcrystalline cellulose: A combined laser induced optoacoustic spectroscopy, diffuse reflectance flash photolysis and luminescence study**
The Journal of Physical Chemistry A, 2014, 118, 10531-10537
Litman, Y; Rodríguez, H; San Román, E*.