Yair Ezequiel Litman

Place and Date of Birth:	Buenos Aires, Argentina | 16 October 1990
Nationality:	Argentinean and Polish
email:	yl899@cam.ac.uk, yairlitman@gmail.com
Virtual presence	Website, Google Scholar, Orcid, Twitter

Education

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

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

Research Experience

Mid-April 2022 – Current | **Research Associate (Walter Benjamin Fellow)**
Yusuf Hamied Department of Chemistry, University of Cambridge
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 contract at 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 Univertät)

Awards & Honors

- 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)
- Acceptance to 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 High-Performance Computing Facility. CSCS National Computer Center (16 Mill core hours, 2018)
- Medal of Honor: 3rd highest GPA (Chemistry, University of Buenos Aires, 2015)

Other Professional activities

Reviewing activities

Reviewer for Nature Communications, Angewandte Chemie, Journal of Chemical Physics, Journal of Physical Chemistry, Journal of chemical theory and computation, Journal of Molecular Liquids, The Journal of Physical Chemistry Letters.

Supervision & mentoring

- Co-supervision of one Master thesis project (University of Cambridge, 2023) (The student was awarded the best theoretical thesis of the year)
- Co-supervision of several projects of 3 PhD students (University of Cambridge, 2022-2024)
- Co-supervision of one project of one PhD student (MPSD, Germany, 2023-2024)

Teaching

- Teaching assistant. (University of Cambridge, 2022)
- Tutor Leader on Practical Exercises on Molecular Dynamics. (Hands-On DFT and Beyond Workshop, Barcelona, 2019)
- Teaching assistant. (University of Buenos Aires, 2015-2016)

Organizer of scientific events

- 3rd n-Aqua Workshop. (Kalamata, Greece 2024)
- Cecam Flagship School. Path Integral Quantum Mechanics. Event website (Tel-Aviv, Israel, 2023)
- Cecam Flagship School. Path Integral Quantum Mechanics: From the Basics to the Latest Developments. Event website (Virtual event, 2021)

Contributions to (scientific) open software

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

Workshops, Meetings and Conferences

Invited Talks

Feb-2024 | **Decoding Aqueous Interfaces with molecular dynamic simulations and surface-specific spectroscopies**
Chemistry Department, Tel Aviv University. Tel Aviv, Israel.

Feb-2024 | **Surface-specific spectroscopy from first principles**
Chemistry Department, Ben Gurion University. Beer Sheva, 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 Institue. 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**
Summerschool 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.

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)

Mar-2024 | **Surface stratification determines the interfacial water structure of simple electrolyte solutions**
Y. Litman, K.Y. Chiang, T. Seki, Y. Nagata, and M. Bonn.
DPG (Deutsche Physikalische Gesellschaft) Spring Meeting. Regensburg, Germany.

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

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

The three most important publications are highlighted in red.

(*=corresponding author, ‡=equal contribution)

1. **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*.
2. **Fully First-Principles Spectroscopy with Machine Learning**
   Journal of Physical Chemistry Letter 2023, 14, 8175
   Litman, Y*; Lan, J; Nagata, Y; Wilkins, D. M*.
3. **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*.
4. **The Is Quantum Vibrational Coupling Important in Water? A spectroscopic perspective**
   (In Preparation)
   Haggard, C; Litman, Y*; Althorpe, S.
5. **Quantum Rates in Dissipative System with Spatially Variable Friction**
   Journal of Chemical Physics 2024, 161, 024110
   Bridge, O; Martinazzo, R; Rossi, M; Althorpe, S; Lazzaroni, P; Litman, Y*.
6. **i-PI 3.0: a flexible and efficient framework for advanced atomistic simulations**
   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.*
7. **Thermal quenching of classical and semiclassical scrambling**
   Phyiscal Review E 2024, 110, L012204
   Sadhasivam, V. G; Hunt, A. C; Meuser, L; Litman, Y, Althorpe, S. C.*
8. **Learning Electronic Polarizations in Aqueous Systems**
   Journal of Chemical Information and Modeling. 2024, 64, 4426
   Jana, A; Shepherd, S; Litman, Y; Wilkins, D. M*.
9. **Tip-enhanced Raman Scattering Imaging Reveals Atomic Scale Chemical Enhancement**
   Journal of Physical Chemistry Letter, *2023, 14, 6850*
   Litman, Y*‡; Bonafe, F‡; Akkoush, A; Appel, H; Rossi, M*.
10. **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.*
11. **Is Unified Understanding of Vibrational Coupling of Water Possible? Hyper-Raman Measurements and Machine Learning Spectra**
    Journal of Physical Chemistry Letter, *2023, 14, 3063*
    Inoue, K‡; Litman, Y‡; Wilkins, D. ; Nagata, Y*; Okuno, M*.
12. **Dissipative Tunneling Rates through the Incorporation of First-Principles Electronic Friction in Instanton Rate Theory II: Benchmarks and Applications**
    Journal of Chemical Physics *2022, 156, 194107*
    Litman, Y*; Pós, E. S; Connor, L. B; Martinazzo, R; Maurer, R. J; Rossi, M*.

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

14. **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*.

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

16. **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*.

17. **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.

18. **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; and Melander, M; Rossi, M; Sakaushi, K; and Saller, M; Schile, A; Sturniolo, S; Trenins, G; Worth, G.

19. **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.

20. **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.

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

22. **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*.

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

24. **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.

25. **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*.

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

27. **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*.