Personal Data

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
Topic: Development of simulation algorithms to simulate non-linear vibrational spectroscopies including nuclear quantum effects. Supervisor: Stuart, Althorpe

Sep 2021 – Feb 2022 | **Postdoctoral Position**
Max Planck Institute for Polymer Research (MPIP)
Topic: Quantum Dynamics at complex aqueous interfaces. Supervisor: Yuki, Nagata and Mischa, Bonn

Aug 2020 – Aug 2021 | **Postdoctoral Position**
Max Planck Institute for the Structure and Dynamics of Matter (MPSD)
Topic: Inclusion of non-adiabatic effects in tunneling rates on metallic systems. Supervisor: Rossi, Mariana

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: Rossi, Mariana. Cosupervisor: Beate, Paulus (Freie Univertät)

Awards

2022 | Poster Prize at Vibrational Spectroscopy GRC, Rhode Island, United States

2019 | Acceptance to 70th Lindau Nobel Laureate Meeting

2019 | Poster Prize at 81st Okazaki Conference, Okazaki, Japan

2018 | Poster Prize at CECAM/Psi-k school on "Path Integral Quantum Mechanics"

Teaching Experience

2023 | **Master thesis co-supervisor**
Yusuf Hamied Department of Chemistry, University of Cambridge
Co-supervision of one Master thesis student.

2022 | **Teaching assistant**
Yusuf Hamied Department of Chemistry, University of Cambridge
Duties: Grading papers, answer questions from students, and carrying out practical lectures. Small groups (2 or 3 students)

Ago-2019
Ago-2017 | **Tutor Leader on Practical Exercises on Molecular Dynamics**
Hands-On DFT and Beyond Workshop
Duties: prepare and test practical exercises; carry out the tutorial on *ab initio* molecular dynamics.

2015-
2016 | **Teaching Assistant**
Graduate position at University of Buenos Aires
Duties: grading papers and exams, answer questions from students, and carrying out lectures. Courses: Analytical Chemistry and Chemical Physics I

2012 | **Teaching Assistant**
Undergraduate position at University of Buenos Aires
Duties: grading papers and exams, answer questions from students, and carrying out lectures. Course: Analytical Chemistry

Grants & Fellowships

2023 | Junior Research Fellowship at Wolfson College

2022 | DAAD travel fellowship to assist the Gordon Research Conference on "Vibrational Spectroscopy"

2021 | Walter Benjamin fellowship awarded by the German Research Foundation (DFG). The Walter Benjamin Programme enables researchers in the postdoctoral training phase to independently conduct their own research project at a location of their choice. Advisor: Stuart Althorpe, University of Cambridge (United Kingdom). Fellowship accepted. Starting date April 2022.

2021 | Newton International Fellowship 2021 (Royal Society). These fellowships are for non-UK scientists who are at an early stage of their research career and wish to conduct independent research in the UK. Advisor: Stuart Althorpe, University of Cambridge (United Kingdom). Fellowship declined.

2018 | DAAD travel fellowship to assist the Gordon Research Conference on "Vibrational Spectroscopy"

2018 | Annual Allocation Time at CSCS National Computer Center. Project: "Tunneling Contributions to the Proton Switching Mechanism of Porphycene on Metallic Surfaces with ab initio Ring Polymer Instantons"

2011 | Eduardo G. Gross: National Academy of Exact Physical and Natural Sciences financial support grant

Computer skills

Programing	Fortran90/95
	Python
	Parallelization (MPI)
Edition	Vi, Latex

Languages

Spanish	Native Speaker
English	Fluent
Hebrew	Basic Knowledge
German	Int. Knowledge

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

Workshops, Meetings and Conferences

Organizer

04-Jun-2021 / 08-Jun-2023 | **Path Integral Quantum Mechanics**
M. Ceriotti, B. Hirshberg, V. Kapil, Y. Litman, T. Markland, and M. Rossi
Tel-Aviv University, Israel.
Event website

14-Jun-2021 / 18-Jun-2021 | **Path Integral Quantum Mechanics: From the Basics to the Latest Developments**
M. Ceriotti, V. Kapil, Y. Litman, T. Markland, and M. Rossi
Total 76 participants. Virtual event.
Event website

Invited Talks

Aug-2023 | **Tip-Enhanced Raman Spectroscopy Made Easy**
FHI-aims users' and developers' meeting. Hamburg, Germany.

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, Gordon Research Seminar. 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-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.

List of Publications: May-2023

(*=corresponding author, ‡=equal contribution)

1. **Surface-Sensitive Spectroscopy with ab initio Accuracy Using Machine Learning**
   arXiv:2305.09321 (Under Review Proceedings of the National Academy of Sciences)
   Litman, Y*; Lan, J; Nagata, Y; Wilkins, D. M*.

2. **Tip-enhanced Raman Scattering Imaging Reveals Atomic Scale Chemical Enhancement**
   arXiv:2211.09475 (Under Review in Journal of Physical Chemistry Letter)
   Litman, Y*; Bonafe, F; Akkoush, A; Appel, H; Rossi, M*.

3. **The Surface of Electrolyte Solutions is Stratified**
   arXiv:2210.01527 (Under Review in Nature Chemistry)
   Litman, Y*; Chiang, K; Seki, T; Nagata, Y; Bonn, M*.

4. **A Hybrid-DFT Study of Intrinsic Point Defects in MX2 (M=Mo, W; X=S, Se) Monolayers**
   In press, Physica Status Solidi A: Applications and Materials Science, DOI:10.1002/pssa.202300180
   Akkoush, A; Litman, Y; Rossi, M.

5. **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*.

6. **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*.

7. **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*.

8. **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*.

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

10. **Temperature Dependence of the Vibrational Spectrum of Porphycene: A Qualitative Failure of Classical-Nuclei Molecular Dynamics**
    Faraday Discussions 2019, 221, 526-546.
    Litman, Y; Behler, J; Rossi, M*.

11. **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.

12. **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.

13. **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.

14. **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.

15. **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*.

16. **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*.

17. **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*.

18. **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*.

19. **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.

20. **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*.

21. **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*.

22. **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*.