
Yair Ezequiel Litman

PERSONAL DATA

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 Universität (Berlin)

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

RESEARCH EXPERIENCE

MID-APRIL 2022 | **Research Associate (Walter Benjamin Fellow)**
CURRENT | 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 | **Postdoctoral Position**
FEB 2022 | Max Planck Institute for Polymer Research (MPIP)
Topic: Quantum Dynamics at complex aqueous interfaces. Supervisor: Yuki, Nagata and Mischa, Bonn

AUG 2020 | **Postdoctoral Position**
AUG 2021 | 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 | **Doctoral Studies**
AUG 2020 | 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 Universität)

TEACHING EXPERIENCE

- | | |
|----------------------|--|
| 2023 | Master thesis co-supervisor
<i>Yusuf Hamied Department of Chemistry, University of Cambridge</i>
Co-supervision of one Master thesis student. |
| 2022 | Teaching assistant
<i>Yusuf Hamied Department of Chemistry, University of Cambridge</i>
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
<i>Hands-On DFT and Beyond Workshop</i>
Duties: prepare and test practical exercises; carry out the tutorial on <i>ab initio</i> molecular dynamics. |
| 2015-
2016 | Teaching Assistant
<i>Graduate position at University of Buenos Aires</i>
Duties: grading papers and exams, answer questions from students, and carrying out lectures. Courses: Analytical Chemistry and Chemical Physics I |
| 2012 | Teaching Assistant
<i>Undergraduate position at University of Buenos Aires</i>
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 <i>ab initio</i> 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](#).

AWARDS

2022		Poster Prize at Vibrational Spectroscopy GRC, Rhode Island, United States
2019		Acceptance to 70 th Lindau Nobel Laureate Meeting
2019		Poster Prize at 81 st Okazaki Conference, Okazaki, Japan
2018		Poster Prize at CECAM/Psi-k school on "Path Integral Quantum Mechanics"

WORKSHOPS, MEETINGS AND CONFERENCES

Organizer

04-Jun-2021		Path Integral Quantum Mechanics
08-Jun-2023		M. Ceriotti, B. Hirshberg, V. Kapil, Y. Litman, T. Markland, and M. Rossi Tel-Aviv University, Israel. Event website
14-Jun-2021		Path Integral Quantum Mechanics: From the Basics to the Latest Developments
18-Jun-2021		M. Ceriotti, V. Kapil, Y. Litman, T. Markland, and M. Rossi Total 76 participants. Virtual event. Event website

Invited Talks

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

- | | |
|----------|--|
| 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. 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. |
| Mar-2018 | Decisive Role of Nuclear Quantum Effects on Surface Mediated Water Dissociation at Finite Temperature
Y. Litman, D. Donadio, M. Ceriotti, M. Rossi
DPG (Deutsche Physikalische Gesellschaft) Spring Meeting. Berlin, Germany. |

List of Publications. Feb-2022.

(* = corresponding author, ‡ = equal contribution)

- 1. Is Unified Understanding of Vibrational Coupling of Water Possible? Hyper-Raman Measurements and Machine Learning Spectra**
(Under Revision in *J. Phys. Chem. Lett.*)
Inoue, K[‡]; Litman, Y[‡]; Wilkins, D. ; Nagata, Y^{*}; Okuno, M^{*}.
- 2. Surface-Sensitive Spectroscopy with ab initio Accuracy Using Machine Learning**
In preparation
Litman, Y^{*}; Lan, J; Nagata, Y; Wilkins, D. M^{*}.
- 3. Tip-enhanced Raman Scattering Imaging Reveals Atomic Scale Chemical Enhancement**
arXiv:2211.09475 (Under Revision in Nano Letters)
Litman, Y^{*}; Bonafe, F; Akkoush, A; Appel, H; Rubio, A; Rossi, M^{*}.
- 4. The Surface of Electrolyte Solutions is Stratified**
arXiv:2210.01527 (Under revision in Nat. Chemistry)
Litman, Y^{*}; Chiang, K; Seki, T; Nagata, Y; Bonn, M^{*}.
- 5. 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^{*}.
- 6. 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^{*}.
- 7. 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^{*}.
- 8. Multidimensional Hydrogen Tunneling in Supported Molecular Switches: The Role of Surface Interactions**
Physical Review Letters 2020, 125, 216001.
Litman, Y^{*}; Rossi, M^{*}.
- 9. 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^{*}.
- 10. 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.
- 11. 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; Gianini, 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.

12. 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.

13. 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.

14. 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*.

15. 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*.

16. 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*.

17. 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*.

18. 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.

19. Positional Isotope Exchange in $\text{HX} \cdots (\text{H}_2\text{O})_n$ ($\text{X} = \text{F}, \text{I}$) Clusters at Low Temperatures

The Journal of Physical Chemistry. A 2016, 120, 7213-7224.

Litman, Y; Videla, P; Rodriguez, J; Laria, D*.

-
20. **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*.
 21. **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*.