

---

# 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

## 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

---

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**  
MARCH 2022 | Max Planck Institute for Polymer Research (MPIP)  
Topic: Quantum Dynamics at complex aqueous interfaces. Supervisor: Yuki, Nagata

AUG 2020 | **Postdoctoral Position**  
SEP 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**  
JULY 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 Univertät)

---

## GRANTS & FELLOWSHIPS

---

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

## INDUSTRY EXPERIENCE

---

JUL 2011	<b>R &amp; D technician and Cyclotron operator</b>
Dec 2014	Bacon Labs, Buenos Aires, Argentina. My duties were divided into two different, clearly separated, roles. As a Cyclotron operator, the operation and maintenance of a Cyclotron (Cyclone 18/9 high current) for 18F-FDG routine production was the main task. In the second place, as an R & D technician, I focused on the design of automatic radiosynthesis for new radiopharmaceutical compounds, such as 18F-Fluorocholine, 13N-Ammonium chloride and 18F-F], Dopa.
JUL 2011	<b>Quality control technician</b>
Dec 2014	Bacon Labs, Buenos Aires, Argentina. Duties: perform microbiological, chemical and physical test of product samples , monitor stages of production; produce reports for quality managers. Used equipment: HPLC Agilent 1100 and Gilson.

## COMPUTER SKILLS

PROGRAMING	Fortran90/95 python Parallelization (MPI)
EDITION	Vi, Latex

## LANGUAGES

SPANISH	Native Speaker
ENGLISH	Fluent
HEBREW	Basic Knowledge
GERMAN	Int. Knowledge

---

## AWARDS

---

- 2022 | Poster Prize at Vibrational Spectroscopy GRC, Rhode Island, United States
- 2019 | Acceptance to 70<sup>th</sup> Lindau Nobel Laureate Meeting
- 2019 | Poster Prize at 81<sup>st</sup> Okazaki Conference, Okazaki, Japan
- 2018 | Poster Prize at CECAM/Psi-k school on "Path Integral Quantum Mechanics"
- 2015 | Medal of Honor: 3<sup>rd</sup> highest GPA in my undergraduate career

## Chemistry Olympiad

- |               |  |
|---------------|--|
| International | Silver Medal (2009), Bronze Medal (2008)                 |
| Iberoamerican | Gold Medal (2008)  |
| Argentinean   | Gold Medal(2008), Gold Medal (2007), Bronze Medal (2006) |

## Argentinean Mathematical Olympiad

- |              |   |
|--------------|---|
| National     | Honorable Mention: 2008, 2007, 2005, 2004 |
| Metropolitan | Honorable Mention: 2008, 2007, 2005       |

## United Nations models

Honorable Mention: MINUBA 2005, MINUBA 2006, UN VIH/SIDA 2006, MINUBA 2007, CAMINU XIII 2007, MINUBA 2008, MINUBA 2009

## Workshops, Meetings and Conferences

### Organizer

- |             |   |
|-------------|---|
| 14-Jun-2021 | <b>Path Integral Quantum Mechanics: From the Basics to the Latest Developments</b>  |
| 18-Jun-2021 | M. Ceriotti, V. Kapil, Y. Litman, T. Markland M. Rossi<br>Main co-organizer of the summer school. Total 76 participants. Virtual event. |

### Invited Talks

- |          |   |
|----------|---|
| Jul-2022 | <b>Surface-Sensitive Spectroscopy with ab initio Accuracy Using Machine Learning</b><br>Vibrational Spectroscopy, Gordon Research Seminar. Rhode Island, United States.                           |
| Jul-2022 | <b>Let the atoms dance with i-PI</b><br>Summerschool on Theoretical Modelling at the Nanoscale, Gordon Research Seminar. Ringberg, Germany.   |
| Nov-2018 | <b>Elucidation of the Quantum Dynamics of Intramolecular Proton Transfer Reaction in Porphycene</b><br>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.

---

## Poster Presentations

- |          |  |
|----------|--|
| Aug-2022 | <b>Surface-Sensitive Spectroscopy with ab initio Accuracy Using Machine Learning</b><br>Y. Litman, K. Chiang, T. Seki, J. Lan, V. Kapil, M. Bonn, D. M. Wilkins, Y. Nagata<br>"Vibrational Spectroscopy, Gordon Research Conference. Rhode Island, United States.                        |
| Mar-2021 | <b>Surface Vibrations Enhance Intramolecular Hydrogen Tunneling in (some) Molecular Switches</b><br>Y. Litman, M. Rossi<br>"Virtual DPG Spring Meeting 2021 of the Surface Science Division", Online event.  |
| Dec-2019 | <b>Elucidating Nuclear Quantum Dynamics of Porphycene: From Gas Phase to Adsorption on Cu(110)</b><br>Y. Litman, M. Rossi<br>"Frontier of Measurement Technologies for Surface Chemistry and Physics in Real-Space, k-Space, and Real-Time", Okazaki, Japan.                             |
| Jul-2018 | <b>Temperature and Tunneling Influence on Intramolecular Double Hydrogen Transfer Reactions</b><br>Y. Litman, T. Kumagai, J. Richardon, M. Rossi<br>Gordon Research Seminar: Vibrational Spectroscopy, New England, United States.   |
| Jun-2018 | <b>Temperature and Tunneling Influence on Intramolecular Double Hydrogen Transfer Reactions</b><br>Y. Litman, T. Kumagai, J. Richardon, M. Rossi<br>Path Integral Quantum Mechanics: From the Basics to the Latest Developments. Cecam, EPFL, Switzerland.                               |
| Jul-2017 | <b>Nuclear Quantum Effects on Surface-Assisted Water Dissociation</b><br>Y. Litman, D. Donadio, M. Ceriotti, M. Rossi<br>Workshop on Understanding Quantum Phenomena with Path Integrals: From Chemical Systems to Quantum fluids and Solids. Trieste, Italy.                            |
| Apr-2015 | <b>Rendimientos cuánticos de formación de triplete en sólidos particulados: estudio comparativo mediante LIOAS, DRLFP y simulaciones numéricas</b><br>Y. Litman, H. B. Rodríguez, E. San Román<br>XIX Congreso Argentino de Fisicoquímica y Química Inorgánica. Buenos Aires, Argentina. |
| Sep-2014 | <b>Fluorescence and Molecular Singlet Oxygen Generation in Thin Films: Phloxine B in Poly(2Hydroxyethyl Methacrylate)</b><br>Y. Litman, H. B. Rodríguez, E. San Román<br>XVI International Congress on Photobiology. Córdoba, Argentina.   |
| Feb-2014 | <b>Fluorescence self quenching and triplet state generation of dyes in constrained media</b><br>Y. Litman, H. B. Rodríguez, S. E. Braslavsky, E. San Román<br>Central European Conference on Photochemistry – CECF. Bad Hofgastein, Austria.   |
| Sep-2013 | <b>A rationale for the development of heterogeneous singlet Oxygen photosensitizers</b><br>Y. E. Litman, H. Rodríguez, S. Braslavsky, E. San Román<br>Congreso de la European Society for Photobiology. Liege, Belgica.  |