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## PERSONAL DATA

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# 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

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

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

## RESEARCH EXPERIENCE

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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 Univertät)

## AWARDS

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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"

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## TEACHING EXPERIENCE

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- 2023 | **Master thesis co-supervisor**  
*Yusuf Hamied Department of Chemistry, University of Cambridge*  
Co-supervision of one Master thesis student. The student was awarded the Norrish Prize for the best Theoretical project.
- 2022 | **Teaching assistant**  
*Yusuf Hamied Department of Chemistry, University of Cambridge*  
Duties: Grading papers, answer questions from students, and carrying out practical lectures. Three small groups (2 or 3 students each)
- Ago-2019 | **Tutor Leader on Practical Exercises on Molecular Dynamics**  
Ago-2017 | *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

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- 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

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## 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](#).

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## WORKSHOPS, MEETINGS AND CONFERENCES

### Organizer

04-Jun-2021	<b>Path Integral Quantum Mechanics</b>
08-Jun-2023	M. Ceriotti, B. Hirshberg, V. Kapil, Y. Litman, T. Markland, and M. Rossi Tel-Aviv University, Israel. <a href="#">Event website</a>
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, and M. Rossi Total 76 participants. Virtual event. <a href="#">Event website</a>

### Invited Talks

Sep-2023	<b>New Insights on Aqueous Electrolyte Interfaces</b> (Selecte poster presentation) The Inaugural Lennard-Jones Centre Meeting: Cambridge, United Kingdom.
Aug-2023	<b>Simulation of Tip-enhanced Raman Spectroscopy</b> FHI-aims users' and developers' meeting. Hamburg, Germany.
Jul-2022	<b>Surface-Sensitive Spectroscopy with ab initio Accuracy Using Machine Learning</b> Vibrational Spectroscopy, Gordon Research Seminar. Rhode Island, United States.
Jul-2022	<b>Let the atoms dance with i-PI</b> Summerschool on Theoretical Modelling at the Nanoscale, Gordon Research Seminar. Ringberg, Germany.
Jun-2022	<b>Tunneling and Zero-Point Energy Effects in Multidimensional Hydrogen Transfer Reactions</b> Lennard-Jones Centre. Cambridge, United Kingdom.
Nov-2018	<b>Elucidation of the Quantum Dynamics of Intramolecular Proton Transfer Reaction in Porphycene</b> Workshop on H-bonding/transfer dynamics of porphycene and its derivatives. Warsaw, Poland.

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### 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. 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.