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 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)

Teaching Experience

2023 | **Part III Supervisor**
Yusuf Hamied Department of Chemistry, University of Cambridge
Co-supervision of one Master thesis student.

2022 | **Supervisor**
Yusuf Hamied Department of Chemistry, University of Cambridge
Duties: Grade students practical exercises. Part 2B A4. Michaelmas Term. 3 student groups.

2022 | **Senior Demonstrator**
Yusuf Hamied Department of Chemistry, University of Cambridge
Duties: Grade students practical exercises. Part 1B A. Michaelmas Term. 2 student groups.

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.

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"

2015 | Medal of Honor: 3rd highest GPA in my undergraduate career

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

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. 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.

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 | **Surface-Sensitive Spectroscopy with ab initio Accuracy Using Machine Learning**
Y. Litman, K. Chiang, T. Seki, J. Lan, V. Kapil, M. Bonn, D. M. Wilkins, Y. Nagata
"Vibrational Spectroscopy, Gordon Research Conference. Rhode Island, United States.

Mar-2021 | **Surface Vibrations Enhance Intramolecular Hydrogen Tunneling in (some) Molecular Switches**
Y. Litman, M. Rossi
"Virtual DPG Spring Meeting 2021 of the Surface Science Division", Online event.

Dec-2019 | **Elucidating Nuclear Quantum Dynamics of Porphycene: From Gas Phase to Adsorption on Cu(110)**
Y. Litman, M. Rossi
"Forefront of Measurement Technologies for Surface Chemistry and Physics in Real-Space, k-Space, and Real-Time", Okazaki, Japan.

Jul-2018 | **Temperature and Tunneling Influence on Intramolecular Double Hydrogen Transfer Reactions**
Y. Litman, T. Kumagai, J. Richardon, M. Rossi
Gordon Research Seminar: Vibrational Spectroscopy, New England, United States.

Jun-2018 | **Temperature and Tunneling Influence on Intramolecular Double Hydrogen Transfer Reactions**
Y. Litman, T. Kumagai, J. Richardon, M. Rossi
Path Integral Quantum Mechanics: From the Basics to the Latest Developments. Cecam, EPFL, Switzerland.

Jul-2017 | **Nuclear Quantum Effects on Surface-Assisted Water Dissociation**
Y. Litman, D. Donadio, M. Ceriotti, M. Rossi
Workshop on Understanding Quantum Phenomena with Path Integrals: From Chemical Systems to Quantum fluids and Solids. Trieste, Italy.

Apr-2015 | **Rendimientos cuánticos de formación de triplete en sólidos particulados: estudio comparativo mediante LIOAS, DRLFP y simulaciones numéricas**
Y. Litman, H. B. Rodríguez, E. San Román
XIX Congreso Argentino de Fisicoquímica y Química Inorgánica. Buenos Aires, Argentina.

Sep-2014 | **Fluorescence and Molecular Singlet Oxygen Generation in Thin Films: Phloxine B in Poly(2Hydroxyethyl Methacrylate)**
Y. Litman, H. B. Rodríguez, E. San Román
XVI International Congress on Photobiology. Córdoba, Argentina.

Feb-2014 | **Fluorescence self quenching and triplet state generation of dyes in constrained media**
Y. Litman, H. B. Rodríguez, S. E. Braslavsky, E. San Román
Central European Conference on Photochemistry – CECP. Bad Hofgastein, Austria.

Sep-2013 | **A rationale for the development of heterogeneous singlet Oxygen photosensitizers**
Y. Litman, H. Rodríguez, S. Braslavsky, E. San Román
Congreso de la European Society for Photobiology. Liege, Belgica.