MARIANO SPIVAK

marspivak@gmail.com ◇ mariano.spivak@lisn.fr ◇ marspivak.gitlab.io/
Paris, France ◇ (+33) 07-6958-5148 ◇ Argentine-Italian

Trained as a computational research scientist, I value good software as it facilitates and speeds up scientific research. As a software developer, I contribute to the scientific community by providing easy-to-use tools that simplify researchers' challenges. Examples include extensions to Visual Molecular Dynamics (VMD), and NAMD in the biophysics community.

EDUCATION

PhD Science and Chemical Technology 2017
MS Theoretical and Computational Chemistry 2012
Universitat Rovira i Virgili (URV). Tarragona, Spain.

EXPERIENCE

Postdoctoral Researcher Universite Paris-Saclay July 2023 -
Advisors: Dr. Nicolas Ferey and Dr. Marc Baaden. LISN and IBPC.
Tasks: Scientific software programmer.
Selected publication product: (`https://doi.org/10.3389/fbinf.2024.1356659`)

Postdoctoral Researcher University of Illinois at Urbana-Champaign July 2018 - June 2023
Advisor: Dr. Emad Tajkhorshid. Beckman Institute, USA.
Tasks: Scientific software programmer. Training coordinator. Workshop lecturer.
Selected publication product: (`https://doi.org/10.1021/acs.jcim.3c00658`)

Doctoral Researcher Universitat Rovira i Virgili October 2012 - January 2017
Advisors: Dr. Coen de Graaf and Dr. Xavier Lopez.
Selected publication product: (`https://doi.org/10.1002/jcc.23672`)

Visiting Researcher at University of Minnesota August - November 2015
Advisor: Dra. Laura Gagliardi. Department of Chemistry. Minneapolis, USA. March - June 2016
Selected publication product: (`http://doi.org/10.1021/acs.jpca.6b10933`)

Visiting Researcher at University of Oxford March - June 2014
Advisor: Dr. John E. McGrady. Inorganic Chemistry Lab. Oxford, UK.
Selected publication product: (`https://doi.org/10.1016/j.ica.2014.08.061`)

SKILLS

- Scientific communication: Lecturer at university courses and conferences.
- Computational Chemistry: Electronic structure calculations with ORCA, Molcas, Gaussian.
- Computational Biophysics: Preparation and analysis of molecular dynamics with VMD, NAMD.
- Programming: Method development with C^{++}/C#, Tcl/Tk and Python. OpenXR.
- Public repository: `https://gitlab.com/marspivak`.
- Courses in Unity, Java Data Structures and Performance and Machine Learning.
- Fluent in English and Spanish, intermediate in French.

OTHER PUBLICATIONS

S. Marru, M. Pierce, B. Plale, S. Pamidighantam, D. Wannipurage, M. Christie, I. Ranawaka, E. Abeysinghe, R. Quick, E. Tajkhorshid, S. Koric, J. Basney, **M. Spivak** et al. Cybershuttle: An End-to-End Cyberinfrastructure Continuum to Accelerate Discovery in Science and Engineering. In Practice and Experience in Advanced Research Computing (PEARC '23). (`https://doi.org/10.1145/3569951.3593602`)

M. Spivak, C. de Graaf, V. Arcisauskaite and X. López. Gating the conductance of extended metal atom chains: a computational analysis of $Ru_3(dpa)_4(NCS)_2$ and $[Ru_3(npa)_4(NCS)_2]$. Physical Chemistry Chemical Physics, Advance Article (2021). (`https://doi.org/10.1039/D1CP02429A`)

M. Spivak, X. López and C. de Graaf. Trends in the Bond Multiplicity of Cr_2, Cr_3, and Cr_2M (M = Zn, Ni, Fe, Mn) Complexes Extracted from Multiconfigurational Wave Functions. The Journal of Physical Chemistry A, 123 (8), 1538-1547 (2019). (`https://doi.org/10.1021/acs.jpca.8b10124`)

M. Spivak, V. Arcisauskaite, X. López and C. de Graaf. Backbone Flexibility of Extended Metal Atom Chains. Ab Initio Molecular Dynamics for $Cr_3(dpa)_4X_2$ (X = NCS, CN, NO3) in gas and crystalline phases. Dalton Transactions, 46, 15487-15493 (2017).
(`https://doi.org/10.1039/C7DT03520A`)

M. Spivak, V. Arcisauskaite, X. López, J. E. McGrady and C. de Graaf. A Multiconfigurational Approach to the Electronic Structure of Trichromium Extended Metal Atom Chains. Dalton Transactions, 46, 6202-6211 (2017). (`https://doi.org/10.1039/C7DT01096F`)

V. Arcisauskaite, D. Fijan, **M. Spivak**, C. de Graaf and J. E. McGrady. Biradical character in the ground state of $[Mn@Si_{12}]^+$: a DFT and CASPT2 study. Physical Chemistry Chemical Physics, 18, 24006-24014 (2016). (`https://doi.org/10.1039/C6CP03534E`)

CONFERENCES PRESENTATIONS, AWARDS AND FELLOWSHIPS

Oral Presentations at American Chemical Society National Meetings.
San Francisco (Online), USA. August 2020
San Diego, USA. August 2019
Boston, USA. August 2015

Oral Presentation at JUJOLS Workshop and Conference on Molecular Magnetism.
Tortosa, Spain. May 2017
Bages, France. June 2015
Mulheim an der Ruhr, Germany. January 2014

Poster Presentation at 8th MQM conference. June 2016
Uppsala University. Uppsala, Sweden.

Oral Presentation at Hammes-Schiffer's group. April 2016
Univeristy of Illinois at Urbana-Champaign. Urbana-Champaign, USA.

Poster Presentation at All Hands Meeting. October 2015
Inorganic Catalyst Design Center. St. Paul, USA.

Poster Presentation at COST Meetings CM1305/CM1002
Second Scientific Workshop. Marseille, France. January 2015
Advances in Computational Spectroscopy. Bratislava, Slovakia. October 2014

Poster Presentation at XIV European SummerSchool September 2013
Quantum Chemistry. Sicily, Italy.

Fellowship for International Students of Master Degree. URV. September 2011