Maximilián Lamanec, Ph.D

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Research Interests

I am an early-career researcher in computational chemistry at the Institute of Organic Chemistry and Biochemistry (IOCB), where I focus on non-covalent interactions and excited states. I have a long-term interest in various computational methods to describe complex systems. My ultimate goal is to secure an independent research position and carry out high-profile fundamental research in electronic structure theory, with a focus on calculations of non-covalent interactions and excited states and close collaboration with experimental groups to correlate theoretical results with experimental observations.

During my graduate studies with Prof. Juraj Kuchár and Prof. Vojtěch Kubíček, I specialized in inorganic chemistry. I later moved to IOCB to work under Prof. Pavel Hobza, where I studied dative bond systems and non-covalent interactions. This position allowed me to directly correlate theoretical results with experimental data and collaborate with Prof. Pavel Jelínek, Prof. Martin Dračínský, Prof. Radek Zbořil, and Prof. Svatopluk Civiš. Currently, I am an independent and enthusiastic postdoctoral researcher with research interests primarily in post-Hartree-Fock methods, multireference calculations of excited states and core-excited states and relativistic effects.

Education

Ph.D. in Physical Chemistry
Palacký University, Olomouc, Czech Republic
Thesis: *From Theory to Experiment: A Computational Chemistry Perspective on Dative Bond and Non-Covalent Interactions*
Advisor: prof. Ing. Pavel Hobza, DrSc., FRSC, dr. h. c.
Co-advisor: RNDr. Dana Nachtigallová, PhD.
Date: 14th June 2024

M.Sc. in Inorganic Chemistry *with honours*
Pavol Jozef Šafárik University, Košice, Slovakia
Thesis: *Halogen Bond in Nano and Bio Systems*
Advisor: doc. RNDr. Juraj Kuchár, PhD.
Co-advisor: prof. Ing. Pavel Hobza, DrSc., FRSC, dr. h. c.
Date: 24th May 2019

B.Sc. in Chemistry
Pavol Jozef Šafárik University, Košice, Slovakia
Thesis: *Intermolecular interactions in coordination compounds*
Advisor: doc. RNDr. Juraj Kuchár, PhD.
Date: 30th August 2017

Research Experience

Postdoctoral Researcher
Pavel Hobza Group, Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic
Dates: 2024 – Present

Junior Researcher
Modelling for Nanotechnologies Lab, IT4Innovations National Supercomputing Center, Ostrava, Czech Republic
Dates: 2021 – Present

Ph.D Researcher
Pavel Hobza Group, Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic
Dates: 2019 – 2024

Visiting student
Department of Physical and Theoretical Chemistry at prof. Michal Pitoňák, Comenius University, Bratislava, Slovakia
Dates: May 2022

Visiting student
Kevin Riley Group, Xavier University of Lousiana, New Orleans, USA
Dates: January – March 2022

Visiting student
Department of Inorganic Chemistry, Charles university, Prague, Czech Republic
Dates: January – July 2017

Awards & Grants

Jean-Marie Lehn Prize for Chemistry, 2025.
Werner von Siemens Award for Best Result of Basic Research, 2021.
Palacký University, Faculty of Science Dean´s Award, 2nd place, 2022.
Palacký University, Student Grant received each year throughout my PhD studies (IGA PrF_2020_022, IGA_PrF_2021_031, IGA_PrF_2022_019, IGA_PrF_2023_018, IGA_PrF_2024_017)

Mentoring

Jitka Zienrtová, *Undergraduate student*, 2023-present
Anna Mašínová, *Summer internship*, Summer 2019; *Undergraduate student*, 2020-2021
Karolína Singerová, *Summer internship*, Summer 2019, Summer 2020

Conferences

ICNI 2019, Lisbon, Portugal
Hydride···π-hole H-bond
Poster

WATOC 2022, Vancouver, Canada
Non-symmetric distribution of electron density at Br atom (σ-hole) in tetrakis(4-bromophenyl) methane
Poster

Skills

Computational Chemistry: Orca, Q-Chem, Molpro, Molcas, Psi4, Turbomole, Dirac, PySCF, NWChem, Gaussian, NBO.
Programming: Python
Languages: English (fluent), Slovak (native)

References

Prof. Pavel Hobza

Distinguished Chair
Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic
Email: pavel.hobza@uochb.cas.cz

Prof. Kevin Riley
Interdisciplinary Research Group (IRG-2): Ionic Gel/solid Interface
Xavier university of Louisiana, New Orleans, USA
Email: kriley3@xula.edu

Prof. Michal Pitoňák
Department of Physical and Theoretical Chemistry
Comenius University, Bratislava, Slovakia
Email: michal.pitonak@uniba.sk

Prof. Michal Otyepka
Head of NANO Lab
IT4Innovations National Supercomputing Center, Ostrava, Czech Republic
Email: michal.otyepka@vsb.cz

Dr. Dana Nachtigallová
Senior Researcher
Institute of Organic Chemistry and Biochemistry, Prague, Czech Republic
Email: dana.nachtigallova@uochb.cas.cz

First Author Publications

1. **Lamanec, M.**†, Lo, R.†, Nachtigallová, D., Bakandritsos, A., Mohammadi, E., Dračínský, M., Zbořil, R., Hobza, P., and Weizhou, W. "The Existence of a N→C Dative Bond in the C_{60}–Piperidine Complex," *Angewandte Chemie International Edition*, **2020**, 59(40), 1942-1950. doi:10.1002/anie.202012851
Impact factor: 16.8; Quartile: Q1

2. Lo, R.†, **Lamanec, M.**†, Weizhou, W., Manna, D., Bakandritsos, A., Dračínský, M., Zbořil, R., Nachtigallová, D., and Hobza, P. "Structure-directed formation of the dative/covalent bonds in complexes with $C_{70}\cdots$piperidine," *Physical Chemistry Chemical Physics*, **2021**, 23, 4365-4375. doi:10.1039/D0CP06280D
Impact factor: 3.9; Quartile: Q1

3. Lo, R.†, Manna, D.†, **Lamanec, M.**†, Wang, W., Bakandritsos, A., Dračínský, M., Zbořil, R., Nachtigallová, D., and Hobza, P. "Addition Reaction between Piperidine and C_{60} to Form 1,4-Disubstituted C_{60} Proceeds through van der Waals and Dative Bond Complexes: Theoretical and Experimental Study," *Journal of the American Chemical Society*, **2021**, 143, 10930-10939. doi:10.1021/jacs.1c01542
Impact factor: 16.4; Quartile: Q1

4. Mallada, B.†, Gallardo, A.†, **Lamanec, M.**†, De La Torre, B., Špirko, V., Hobza, P., and Jelínek, P. "Real-space Imaging of Anisotropic Charge of σ-hole by Means of Kelvin Probe Force Microscopy,"

Science, **2021**, 374, 863-867. doi:10.1126/science.abk1479
Impact factor: 63.8; Quartile: Q1

5. Civiš, S.[†], **Lamanec, M.**[†], Špirko, V., Kubišta, J., Špeťko, M., and Hobza, P. "Hydrogen Bonding with Hydridic Hydrogen – Experimental Low-Temperature IR and Computational Study: Is a Revised Definition of Hydrogen Bonding Appropriate?" *Journal of the American Chemical Society*, **2023**, 145, 8550-8559. doi:10.1021/jacs.3c00802
Impact factor: 14.5; Quartile: Q1

6. Mallada, B.[†], Ondráček, M.[†], **Lamanec, M.**[†], Gallardo, A., Jiménez-Martín, A., de la Torre, B., Hobza, P., and Jelínek, P. "Visualization of π-Hole in Molecules by Means of Kelvin Probe Force Microscopy," *Nature Communications*, **2023**, 14, 4954. doi:10.1038/s41467-023-40593-3
Impact factor: 14.7; Quartile: Q1

7. **Lamanec, M.**, Zienertová, J., Špeťko, M., Nachtigallová, D., and Hobza, P. "Similarities and Differences of Hydridic and Protonic Hydrogen Bonding," *ChemPhysChem*, **2024**, 25, e202400403. doi:10.1002/cphc.202400403
Impact factor: 2.3; Quartile: Q2

8. **Lamanec, M.**, Civiš, S., and Hobza, P. "On the similar spectral manifestations of protonic and hydridic hydrogen bonds despite their different origin," *Communications Chemistry*, **2024**, 7, 224. doi:10.1038/s42004-024-01334-9
Impact factor: 5.9; Quartile: Q1

9. Manna, D.[†], Lo, R.[†], **Lamanec, M.**[†], Pavlišová, J., Socha, O., Dračínský, M., and Hobza, P. "Beyond Deshielding: NMR Evidence of Shielding in Hydridic and Protonic Hydrogen Bonds," *Journal of Chemical Theory and Computation*, **2025**, 21, 15, 7495-7502. doi:0.1021/acs.jctc.5c00870
Impact factor: 5.5; Quartile: Q1

10. **Lamanec, M.**, Špirko, V., Civiš, S., and Hobza, P. "Blue-Shifting Hydridic Hydrogen Bonds," *Submitted.*

[†]These authors contributed equally to this work and can be considered as the first author.

Contributing Author Publications

1. Lo, R., Manna, D., **Lamanec, M.**, Dračínský, M., Bouř, P., Wu, T., Bastien, G., Kaleta, J., Miriyala, V. M., Špirko, V., Mašínová, A., Nachtigallová, D., and Hobza, P. "The Stability of Covalent Dative Bond Significantly Increases with Increasing Solvent Polarity," *Nature Communications*, **2022**, 13, 2107. doi:10.1038/s41467-022-29806-3
Impact factor: 16.6; Quartile: Q1

2. Lo, R., Mašínová, A., **Lamanec, M.**, Nachtigallová, D., and Hobza, P. "The unusual stability of H-bonded complexes in solvent caused by greater solvation energy of complex compared to those of isolated fragments," *Journal of Computational Chemistry*, **2023**, 44(3), 329. doi:10.1002/jcc.26928
Impact factor: 3.4; Quartile: Q1