Pierpaolo Morgante

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Professional Experience

Institute of Physics (IOP) Publishing
(August 2023 – Present)
Subject commissioning editor working across the journal portfolio: applications of machine learning to the physical, chemical, and life sciences.

University at Buffalo, State University of New York
(May 2021 – July 2023)
Post-doctoral researcher in the Department of Chemistry
Advisor: Prof. Jochen Autschbach

Education

Florida Institute of Technology
(August 2017 –May 2021)
Ph.D. student in Theoretical and Computational Chemistry. Graduation date: May 1st, 2021.
Dissertation: "Development of diagnostic tools and analysis of the density functional theory zoo."
Advisor: Dr. Roberto Peverati
Committee: Dr. A. B. Brown, Prof. N. Nesnas, Dr. J. C. Perez, Prof. D. A. Knight, Dr. R. Peverati (Chair)

University of Turin, School of Natural Sciences, Department of Chemistry
Master of Science in Advanced Chemical Methodologies, Curriculum Structure.
Graduation date: December 15th, 2016. Summa cum laude, first of the class.
Dissertation: "Computational study of the stereoselectivity in the alkylation of cyclic silyl enol ethers by diarylmethylium salts."
Advisors: Dr. Giovanni Ghigo, Dr. Margherita Barbero, Prof. Bartolomeo Civalleri.

Conservatorio Statale di Musica "G. Verdi" di Torino
T. S. M. in Saxophone (Italian equivalent of a bachelor of Arts).
Graduation date: March 20th, 2017. Summa cum laude.

University of Turin, School of Natural Sciences, Department of Chemistry
Bachelor of Science in Chemistry.
Graduation date: April 10th, 2014. Summa cum laude.
Dissertation: "Copper catalyzed dehydrogenative cross-coupling of tertiary amines."
Advisor: Dr. Giovanni Ghigo.

Awards

Outstanding Graduate Student

Awarded on December 1st, 2018 by the Orlando Section of the American Chemical Society.

Outstanding Graduate Student in Chemistry

Awarded in April 2019, March 2020, and April 2021 by the Biomedical and Chemical Engineering and Sciences Department at Florida Institute of Technology.

Physical Chemistry (#RSCPhys) Runner-Up Poster Award

Awarded on March 13th, 2020 by the Royal Society of Chemistry for the poster "The Devil in the Details: What Everybody Should Know When Running DFT Calculations" participating at the 2020 Royal Society of Chemistry Poster (#RSCPoster) Twitter Conference.

Publications

Textbook:

P. Morgante, J. Autschbach, "Molecular Orbitals", American Chemical Society (ACS) "In Focus" series, Washington, D. C. (USA), **2023**.

Journal articles:

21) A. Saju, P. S. Gunasekera, P. Morgante, S. N. MacMillan, J. Autschbach, D. C. Lacy, "Experimental and Computational Determination of a M–Cl Homolytic Bond Dissociation Free Energy: Mn(III)Cl Mediated C–H Cleavage and Chlorination", *J. Am. Chem. Soc.*, **2023**, *145*, 13384–13391.

20) P. Morgante, J. Autschbach, "Strategies to Calculate Fukui Functions and Applications to Radicals with SOMO-HOMO Inversion", *J. Chem. Theory Comput.*, **2023**, *19*, 3929–3942.

19) P. Sumsalee, P. Morgante, G. Pieters, J. Crassous, J. Autschbach, L. Favereau, "Negative solvatochromism and sign inversion of circularly polarizedluminescence in chiral exciplexes as a function of solvent polarity", *J. Mat. Chem. C.*, **2023**, *11*, 8514–8523.

18) P. Morgante, J. Autschbach, "Density-Corrected Density Functional Theory for Molecular Properties", *J. Phys. Chem. Lett.*, **2023**, *14*, 4983–4989.

17) P. Morgante, R. Peverati, "Comparison of the Performance of Density Functional Methods for the Description of Spin States and Binding Energies of Porphyrins", *Molecules*, **2023**, *28*, 3847.

16) K. Dhbaibi, P. Morgante, N. Vanthuyne, J. Autschbach, L. Favereau, J. Crassous, "Low Temperature Luminescence in Organic Helicenes: Singlet Versus Triplet State Circularly Polarized Emission", *J. Phys. Chem. Lett.*, **2023**, 14, 1073–1081.

15) B. C. Baciu, P. J. Bronk, T. de Ara, R. Rodriguez, P. Morgante, N. Vanthuyne, C. Sabater, C. Untiedt, J. Autschbach, J. Crassous, A. Guijarro, "Dithia[9]helicenes: Molecular Design, Surface Imaging, and Circularly Polarized Luminescence with Enhanced Dissymmetry Factors", *J. Mater. Chem. C*, **2022**, *10*, 14306–14318.

14) S. Paul, P. Morgante, S. N. MacMillan, J. Autschbach, D. Lacy, "Hydrogenative catalysis with three-coordinate zinc complexes supported with PN ligands is enhanced compared to PNP analogs", *Chem. Eur. J.*, **2022**, *28*, e202201042.

13) P. Morgante, H. D. Ludowieg, J. Autschbach, "Comparative Study of Vibrational Raman Optical Activity with Different Time-Dependent Density Functional Approximations: The VROA36 Database", *J. Phys. Chem. A*, **2022**, *126*, 2909–2927.

12) R. Wehmschulte, B. Bayliss, S. Reed, C. Wesenberg, P. Morgante, R. Peverati, S. Neal, C. Chouinard, D. Tolosa, D. Powell, "Zinc Ammonio-dodecaborates: Synthesis, Lewis Acid Strength and Reactivity", *Inorg. Chem.*, **2022**, *61*, 7032–7042.

11) P. Morgante, C. Deluca, T. E. Jones, G. J. Aldrich, N. Takenaka, and R. Peverati, "Steps toward Rationalization of the Enantiomeric Excess of the Sakurai–Hosomi–Denmark Allylation Catalyzed by Biisoquinoline N,N'-Dioxides Using Computations", *Catalysts*, **2021**, *11*, 1487.

10) P. Morgante, C. Guruge, Y. P. Ouedraogo, N. Nesnas, R. Peverati, "Competition between cyclization and unusual Norrish type I and type II nitro-acyl migration pathways in the photouncaging of 1-acyl-7-nitroindoline revealed by computations", *Scientific Reports*, **2021**, 11, 1396.

9) E. Epifanovsky *et al.,* "Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package ", *J. Chem. Phys.,* **2021**, 185, 084801.

8) P. Morgante, R. Peverati, "CLB18: A New Structural Database with Unusual Carbon–Carbon Long Bonds", *Chem. Phys. Lett.*, **2021**, 765, 138281.

7) P. Morgante, R. Peverati, "The devil in the details: A tutorial review on some undervalued aspects of density functional theory calculations", *Int. J. Quantum. Chem.*, **2020**, 120, e26332.

6) P. Morgante, B. Captain, C. D. Chouinard, R. Peverati, N. Takenaka, "Synthesis of electrophilic N-heterocyclic carbenes based on azahelicene", *Tetrahedron Lett.*, **2020**, 61, 152143.

5) P. Morgante, R. Peverati, "Statistically representative databases for density functional theory via data science", *Phys. Chem. Chem. Phys.*, **2019**, 21, 19092–19103.

4) P. Morgante, R. Peverati, "ACCDB: A collection of Chemistry DataBases for broad computational purposes", *J. Comput. Chem.*, **2019**, 40, 839–848.

3) P. Morgante, S. Dughera, G. Ghigo, "Aerobic $CuCl_2$-catalyzed dehydrogenative cross-coupling of tertiary amines. A combined computational and experimental study", *J. Phys. Chem. A*, **2019**, 123, 2796–2814.

2) C. Reep, P. Morgante, R. Peverati, N. Takenaka, "Axial-Chiral Biisoquinoline N,N'-Dioxides Bearing Polar Aromatic C-H Bonds as Catalysts in Sakurai-Hosomi-Denmark Allylation", *Org. Lett.,* **2018**, 20, 5757–5761.

1) M. Barbero, S. Cadamuro, S. Dughera, G. Ghigo, D. Marabello, P. Morgante, "Efficient alkylation of cyclic silyl enol ethers by diarylmethylium salts", *Tetrahedron Lett.*, **2016**, 57, 4758–4762.

Conference papers:

1. G. Ghigo, S. Dughera, P. Morgante, "The mechanism of the aerobic Cu catalyzed oxidative cross-coupling of tertiary amines. An experimental and computational study", 36th conference of the Organic Chemistry Division of the Italian Chemical Society; Bologna, September 13th–September 17th, **2015**.
2. P. Morgante, R. Peverati, "The Devil in the Details: What Everybody Should Know When Running DFT Calculations", 6th Royal Society of Chemistry Poster (#RSCPoster) Conference, March 3rd–March 4th, **2020**.
3. P. Morgante, R. Peverati, "Assessment of more than 200 Density Functional Approximations for Binding Energies and Spin States of Porphyrins", 257th American Chemical Society National Meeting; Orlando (FL), March 31st–April 4th, 2019. Presented on April 2nd, **2019**.
4. "Strategies to calculate Fukui functions and applications to radicals with SOMO-HOMO inversion", Fall 2023 National Meeting of the American Chemical Society; San Francisco (CA), August 13th–August 17th. Scheduled for August 15th.

Presentations (least-to-most recent)

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1. University of New South Wales, Sydney, Australia: "The devil in the details: A tutorial review on some undervalued aspects of density functional theory calculations." April 21st, 2020. Host: Dr. Laura McKemmish.
2. Department of Chemistry and Chemical Biology, Northeastern University, USA: "Visiting the density functional theory zoo: Databases of chemical data and how to uncage glutamate." January 15th, 2021. Host: Dr. Sijia Dong.
3. Department of Chemistry, University of Turin, Italy: "The Devil in the details: A presentation about some undervalued aspects of Density Functional Theory calculations." February 26th, 2021. Host: Dr. Giovanni Ghigo.
4. Lecturer on the online platform JAWS (Just Another Chemistry Webinar Series): "The Devil in the details: A presentation about some undervalued aspects of Density Functional Theory calculations." March 2nd, 2021.
5. Lecturer (online) for the Material Science course at the University of Turin: "The Devil in the details: A presentation about some undervalued aspects of Density Functional Theory calculations." May 13th, 2021. Host: Prof. B. Civalleri.
6. "Undervalued Aspects of Density Functional Theory Calculations in Chemical Education", Fall 2023 National Meeting of the American Chemical Society; San Francisco (CA), August 14th, 2023.
7. "Density-Corrected Density Functional Theory Calculations of Dipole Moments, Polarizabilities and Electric Field Gradients", Fall 2023 National Meeting of the American Chemical Society; San Francisco (CA), August 17th, 2023.
8. Department of Chemistry, Florida Institute of Technology, Melbourne (FL), United States: "How to get (your research) published". December 14th, 2023. Host: Dr. Roberto Peverati.