Pierpaolo Morgante

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Education

Florida Institute of Technology
(August 2017 – present; Expected Graduation: May 2021)
Ph.D. student in Theoretical and Computational Chemistry.
Advisor: Dr. Roberto Peverati

University of Turin, School of Natural Sciences
Master's Degree in Advanced Chemical Methodologies, Curriculum Structure, earned on December 15th, 2016. Summa cum laude, first of the class.
Thesis: "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, Bachelor of Arts earned on March 20th, 2017. Graduated with honors.

University of Turin, School of Natural Sciences
Bachelor's degree in Chemistry earned on April 10th, 2014. Summa cum laude.
Thesis: "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 on April 11th, 2019 by the Biochemical 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.

Outstanding Graduate Student in Chemistry.

Awarded in March 2020 by the Biochemical and Chemical Engineering and Sciences Department at Florida Institute of Technology.

Publications

Journal articles:

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.

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

R. J. Wehmschulte, B. Bayliss, S. Reed, C. Wesenberg, P. Morgante, R. Peverati, D. Tolosa, D. R. Powell, "Zinc Ammonio-dodecaborates: Synthesis, Lewis Acid Strength and Reactivity", *in preparation*.

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.

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.

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

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

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.

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.

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:

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**.

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**.

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**.