Federica Maschietto

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Summary

Computational chemist experienced in excited state chemistry, particularly interested in the photochemistry and photo-reactivity of metal-organic complexes and organic systems, with applications, from energetics to medicinal chemistry. Current work focusses on the development and application of theoretical approaches, rooted on density functional theory, for the accurate description of excited state potential energy surfaces involving profound structural reorganization.
Frequent speaker, with excellent vulgarization skills. Structured and creative enough to solve most challenging problems independently, given the necessary knowledge. Fast learner, with proven ability to enter a new field and leverage previous knowledge. Convinced team worker, when it comes to interdisciplinary tasks.

Key Skills

- Expert in TD-DFT, Excited States Modelling
- Proficient user of a variety of quantum chemical and visualization software (Gaussian, Dalton, Molpro, VMD, PyMol, …)
- AWK, Bash Scripting Language
- Python Programming Language
- Teaching, framing experience
- Collaboration with experimentalists

Experience

Sep 2016 – Present **PhD Candidate at Chimie Paris Tech – Paris, France**

Under the supervision of Dr. Ilaria Ciofini, within the group led by Professor Carlo Adamo. Research focussed on the development of new methodologies for the rationalization of the photochemical properties of organic and inorganic molecular systems. Research mainly oriented to model excited state properties and reaction pathways of light-responsive molecular system such as photo-switches and transition metal complexes. Required to work independently, in collaboration with other members of the group and with many external experimental chemists, for which it is required to create brief, high quality reports, explain findings and discuss their implications. Given the opportunity to work on a variety of other projects, including investigations of systems of biological relevance and metal complexes applied in photodynamic therapy. Currently have teaching duties which span three separate courses concerning molecular modelling and quantum mechanical theory, totalling approximately 50 hours per year.

Oct-May 2016 **Joint Research intern at UPMC Paris - FU Berlin, Germany**

Under the supervision of Prof. Dr Beate Paulus in Berlin took charge of a project aimed at the theoretical investigation of the nitrene functionalization of C_{60} fullerene and carbon nanotubes. Became familiar with ab initio QM methods chemical approaches, from density functional theory to wavefunction and semiempirical methods. Based on academic merit and the strength of the research proposal, I was awarded a Promos Scholarship of €1500 to visit Dr. Peter Reinhardt at the LCT in Paris, under the guidance of which I finalized my master project. Despite the short time frame of the internship, parts of this work were later included in two publication, in *Nature Communications* and *RSC Advances.*

Apr-Aug 2015 **Research intern Bayer Health – Berlin,**

Project aimed at the development of a *in Silico* model to predict mutagenicity of aromatic amines, based on the correlation between chemical fragments and their response to the Ames test. Became familiar with big data manipulation, and statistical analysis. Simulations were performed using an in-house suite of programs and data analysis was carried out with tools I designed using the bash scripting Python programming languages coupled with the Pipeline Pilot program.

Set 2015 - May 2016 **Mentoring activity at FU Berlin**

Mentoring activity for international students entering the first year of a Bachelor/Master program at FU

Education

Sep 2013 – May 2016 **Masters in Chemistry –** Grade 1,3 (top 5%)
Freie Universität Berlin, Germany

Higher tuition in the different fields of the theoretical chemistry and the state-of-art techniques for modelling chemical systems. Fundamentals of quantum chemistry including Hartree-Fock, Post Hartree- Fock as well as Density Functional based methods and their application in the study of molecular systems, both from a time dependent and time independent perspective. Complete overview of modern aspects of spectroscopy, advanced organic synthesis and stereoselective chemistry.

Sep 2010 – July 2013 **Laurea Triennale in Chimica e Chimica dei Materiali** (Bachelor Degree),
110/110 Cum Laude
Alma Mater Studiorum Bologna, Italy

Sep 2009 – July 2010 **First year Bachelor Degree in Biological Sciences**,
Average grade 30/30
Alma Mater Studiorum Bologna, Italy

Sep 2004 – July 2009 Liceo Classico Galileo
Florence, IT

Awards

2016	Promos scholarship holder, Internship Université PMC Paris
2014-2015	Deutsche Akademischer Austausch Dienst (DAAD) Scholarship holder

Publications

Following excited state in molecular systems using density-based indexes: a dual emissive system as a test case,
F Maschietto†, A Perfetto†,I Ciofini, Submitted to Journal of Photochemistry and Photobiology A.

A Ru(II) Polypyridyl Complex Bearing Aldehyde Functions as a Versatile Synthetic Precursor for Long-Wavelength Absorbing Photodynamic Therapy Photosensitizers,
J Karges, F Heinemann, F Maschietto, M Patra, O Blacque, I Ciofini, B Spingler, and G Gasser,
Bioorganic & Medicinal Chemistry, 2019, 27 (12), 2666-75. [full text link].

Using density-based indexes to characterize excited states evolution
F Maschietto†, J Sanz-Garcia, M Campetella,
Journal of Computational Chemistry, **2019**, 40, 650-656. [full text link]

Design of dendritic core carbazole-based hole transporting materials for efficient and stable hybrid perovskite solar cells
TT Bui, M Ulfa, F Maschietto, A Ottochian, MP Nghiêm, I Ciofini, F Goubard, T Pauporté
Organic Electronics, **2018**, 60, 22-30. [full text link]

How are the charge transfer descriptors affected by the quality of the underpinning electronic density?
F Maschietto†,, M Campetella, MJ Frisch, G Scalmani, C Adamo, I Ciofini [full text link]
Journal of Computational Chemistry, **2018**, 39 (12), 735-742.

Using Density Based Indexes and Wave Function Methods for the Description of Excited States: Excited State Proton Transfer Reactions as a Test Case
J Sanz García, F Maschietto, M Campetella, I Ciofini
The Journal of Physical Chemistry A, **2018**, 122 (1), 375-382. [full text link]

Charge transfer excitations in TDDFT: A ghost-hunter index
M Campetella, F Maschietto, MJ Frisch, G Scalmani, I Ciofini, C Adamo
Journal of Computational Chemistry, **2017**, 38 (25), 2151-2156, [full text link]

Preserving π-conjugation in covalently functionalized carbon nanotubes for optoelectronic applications
A Setaro, M Adeli, M Glaeske, D Przyrembel, T Bisswanger, G Gordeev, F Maschietto, A Faghani, B. Paulus, M Weinelt, R Arenal, R Haag and S Reich
Nature Communications, **2017**, 8, 14281. [full text link]

Functionalization of fullerene at room temperature: toward new carbon vectors with improved physicochemical properties
Z Beiranvand, A Kakanejadifard, IS Donskyi, A Faghani, Z Tu, A Lippitz, P Sasanpour, F Maschietto, B Paulus,
RSC Advances 6, **2017**, (114), 112771-112775.

† First Author

Conference Contributions

Journé Théorie Modélisation Simulation
23-25 May 2018, Paris, Oral Communication

2nd Scientific day of the i-CLeHS
3 July 2018, Paris, Oral Communication

Molecular Electronic Structure Conference (MESM)
28-31 August 2018, Metz, Oral Communication

Second European Symposium on Chemical Bonding (ESCB2)
4-7 September 2018, Oviedo, Oral Communication

Excited State Complex Systems (ESCS)
21-25 November 2016, Paris, Poster Presentation

International Conference of Chemists of Latin Expression, (Chitel)
3-7 July 2017, Paris, Poster Presentation

International Conference on Photochemistry (ICP)
16-21 July 2017, Strasbourg, Poster Price

Rencontres des Chimistes Théoriciens Francophones (RCTF)
8-12 October 2018, Toulouse, France, Poster Presentation

Additional Skills

Native Italian speaker
Fluent English speaker, proficient at reading and writing
Fluent French speaker
Fluent German speaker