

# Marco Campetella

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## Personal Information

- Date of Birth: [REDACTED]
- Place of Birth: [REDACTED]

## Academic positions

### Dr. Matteo Calandra's group, CNRS

Paris

- Postdoctoral Researcher

September 2018–Ongoing

I am characterizing both electronic and structural properties of different kinds of 2D materials. At the moment I am focusing my attention on Bernal stacked bilayer graphene, the Misfit Layer Compound  $\text{LaNb}_2\text{LaS}$  and Perovskite oxides. Moreover I am studying anharmonic effects on 1D system, characterizing in a reliable way the charge density waves (CDWs). All of the projects are carried out using both plane wave and Gaussian basis sets.

### Dr. Ilaria Ciofini's group, CNRS

Paris

- Postdoctoral Researcher

September 2016–August 2018

First thing, I focused my attention on the behaviour of the particle-hole distance varying both the acceptor-donor distance (in push-pull systems) and the functionals in TDDFT calculations. Subsequently, I devised two different indexes, the first one to evaluate the particle-hole distance, taking into account only the contributions of a selected group of atoms. The second index is able to detect ghost states in the framework of TDDFT theory. Finally I have devised a new protocol to perform excited states optimization, tracking a specific state characterized by a well defined electronic state.

### Prof. Benedetta Mennucci's group, Università di Pisa

Pisa

- Postdoctoral Researcher

July 2015–July 2016

I have carried out two different projects, the first one regarding the Simulations of Excitonic Absorption and Circular Dichroism Spectra of Proteins and Light harvesting systems. This project involves the study of the influence of structural fluctuations, through Molecular Dynamics trajectories, and of the environment, through continuum or atomistic models, in the simulation of Excited State properties. In the second project a robust and automated protocol for the derivation of sound force field parameters, suitable for condensed-phase classical simulations, is tested and validated on several halogenated hydrocarbons, a class of compounds for which standard force fields have often been reported to deliver rather inaccurate performances. The major strength of the proposed protocol is that all of the parameters are derived only from first principles because all of the information required is retrieved from quantum mechanical data.

## Teaching

### ENSCP Chimie ParisTech

Paris

- Teacher

2018

During my second post doc, I held a Mini-course on quantum chemistry for PhD students: "Principles of Quantum Chemistry".

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During my PhD, I held the position of assistant for both the chemistry and the physics courses for the natural science bachelor degree.

## Education

Roma

### Università "La Sapienza"

October 2011–October 2014

#### Ph.D., Material Science

Dissertation: "Structural studies of ionic liquids by means of X-ray and theoretical methods". Advisor: Prof. Ruggero Caminiti.

During my PhD thesis I focused my attention on the characterization of Ionic Liquids (ILs). Those intriguing systems have acquired a leading position in the field of innovative materials developed in the last twenty years, owing to their remarkable properties that constitute an attractive issue for both academic and industrial communities. One of the key issue to understand the properties of these compounds and to facilitate their use is related to their structure. The nature of the cation-anion interactions and how they determine the structure of the ionic liquids are, therefore a crucial step for their study. In this work, an approach in which experimental techniques are used in combination with theoretical studies was used. The experimental technique that has been mainly used is X-ray diffraction and in a few cases also IR spectroscopy. Classical molecular dynamics (AMBER, DLPOLY) and *ab initio* calculations (CP2K, CPMD) have been used as theoretical methodologies. The use of different methodologies allowed, on the one hand, to have structural experimental data on which to test the accuracy of the simulation models, and, on the other, to study the detailed structure of the systems at a molecular level. One of the most debated topics about the structure of ionic liquids appears to be the presence of a long-range order, pointed out by X-Ray patterns. This theme is further developed in this thesis focusing on a series of ionic liquids with alkyl chain of variable length and studying areas at low diffraction angles both experimentally and theoretically.

#### Mulliken Center

Bonn

#### Visiting Ph.D. Student

March 2013–July 2013

Project: "Study of Ionic Liquids by means Cp2k and TRAVIS softwares". Advisor: Prof. Barbara Kirchner. During this training period I introduced myself in the world of *ab initio* molecular dynamics. Exploiting this computational tool is necessary for a lot of systems, because when strong polarization and many-body effects come into play, it is extremely difficult to provide valuable computational results using a pairwise potentials like those commonly employed by most of classical MD simulation programs. The final goal was the exploration, by means of *ab initio* molecular dynamics, of a sub-set of three different protic ionic liquids. I studied both structural and dynamical information of the liquid state of these compounds, like the hydrogen bond network and the velocity density of state of the atoms.

### Università "La Sapienza"

Roma

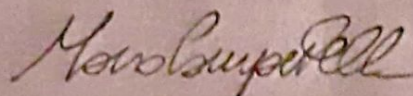
#### Master's Degree, Physics of Matter

September 2009–September 2011

Title: Glue function in superconductor Cuprate: *no biased approach*. Advisor: Prof. Marco Grilli

During my thesis I address the issue of identifying the mediators of effective interactions in cuprates superconductors. Specifically, I use inversion theory to analyze Raman spectra of optimally and overdoped  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  samples. This allows me to extract the so-called glue function without making any *a priori* assumption based on any specific model. I use instead two different techniques, namely the singular value decomposition and a multi-rectangle decomposition. To perform such

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study it was necessary the implementation of the mathematical model in a Fortran90 code, for both the techniques.

Università "La Sapienza"

Roma

◦ Bachelor's Degree, Physics

September 2006–September 2009

Università "La Sapienza"

Roma

◦ Master's Degree, Computational Chemistry

September 2004–September 2006

Title: Electron-molecules scattering: a theoretical approach. Advisor: Prof. F.A. Gianturco

During my thesis I performed the computational studies of the interaction of low-energy electrons with the purine bases of DNA, adenine and guanine, as well as with the associated nucleosides, deoxyadenosine and deoxyguanosine, and the nucleotide deoxyadenosine monophosphate. Their calculations focus on the characterization of the  $\pi^*$  shape resonances associated with the bases and also provide general information on the scattering of slow electrons by these targets. Results are obtained for adenine and guanine both with and without inclusion of polarization effects, and the resonance energy shifts observed due to polarization are used to predict  $\pi^*$  resonance energies in associated nucleosides and nucleotides, for which static-exchange calculations were carried out. They observe slight shifts between the resonance energies in the isolated bases and those in the nucleosides. The theoretical findings (cross-section) were directly compared with the experimental one, in order to endorse the adapted model.

Università "La Sapienza"

Roma

◦ Bachelor's Degree, Chemistry

September 2001–September 2004

## Fellowships

Università "La Sapienza"

Roma

◦ Graduate School "La Sapienza" Ph.D. Fellowship

October 2011–October 2014

CASPUR

Roma

◦ Graduate Fellowship, Material Science

February 2008–July 2009

Topic: "Structural study in aqueous solution of heterocyclic systems such as Pirazole, Triazole and their derivatives". Advisor: Prof. Fabio Raimondo.

During this work the local structure of the hydration of pyrazole has been analysed through static and dynamical microsolvation models described by quantum mechanical methods. Then, a reliable classical force field of pyrazole has been obtained on the basis of the quantum mechanical results and the dynamical properties of aqueous pyrazole solutions have been studied by molecular dynamics simulations. Finally, the structure of pyrazole–water solutions at different concentrations has been investigated by energy dispersive X-ray diffraction and experimental results have been compared to calculations. This comparison provides both a tool for interpretation of experiments and a way to validate the computational protocol.

## Languages

- Italian: native speaker.
- English: fluent.
- French: basic.

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Mario Caspura



## Schools

- January 2020 Computational School on Electronic Excitations in Novel Materials Using the Yambo Code (Trieste, Italy)
- September 2017 European Summer School in Quantum Chemistry (Torre Normanna, Italy)
- August 2015 CECAM 4<sup>th</sup> CP2K Tutorial (Lausanne, Switzerland)
- February 2013 School in Introduction to HPC: parallel computing, CASPUR (Rome, Italy)
- June 2012 School in Introduction to HPC: high performance computing, CASPUR (Rome, Italy)
- May 2012 CECAM Car-Parrinello Molecular Dynamics (CPMD) tutorial: understanding condensed matter and molecular physics (Lausanne, Switzerland)

## Conferences

- April 2018 Oral Presentation at the « ACS » (Boston, U.S.A.) : "Tuned quantification of particle-hole distance in charge-transfer excitations: A revised version of the DCT index".
- March 2017 Oral Presentation at the « TheoBio » (San Sebastian, Spain) : "Charge Transfer Excitations in TDDFT: A Ghost-Hunter Index".
- March 2017 Oral Presentation at the « CMS » (Warwick, U.K.) : "Ghost states in TDDFT : a reliable descriptor for their detection".
- November 2016 Oral Presentation at the « ESCS » (Paris, France) : "Excitonic Approach in Complex Light Harvesting Systems".
- April 2016 Oral Presentation at the « ACS » (San Diego, U.S.A.) : "Simulation of the electronic spectra of LH2 complex of bacteria through a polarizable QM/MM approach".
- March 2013 Poster contribution at the « Winter Modeling » (Modena, Italy) : "Static and Dynamical Properties of Oxirane : an Experimental and Theoretical Approach".

## Computer skills

- **Programming Languages:** very good knowledge of Python, Fortran90, C, Parallel (MPI and OpenMP) coding and shell scripting languages (Bash, Csh).
- **Computational Chemistry Software:** advanced knowledge of Gaussian, Cp2k, CPMD, Amber, Gromacs, DLPOLY and VMD. Good experience with Orca, SSCHA, Crystal and Quantum Espresso.

## Reviews

- Reviewer for the Journal of Chemical Theory and Computation, Spectrochimica Acta Part A, Molecular and Biomolecular Spectroscopy, Physical Chemistry Chemical Physics, Computational and Theoretical Chemistry, The European Physical Journal Plus, International Journal of Quantum Chemistry, Molecular Physics.

## Editor

- Editor for Special Issue "Materials Science and X-Ray Diffraction" for the journal "Symmetry".

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## Theses

- o Coadvisor of the Master Thesis in Computational Chemistry "Geometry optimization of Multicenter Transition Metal clusters through Extended Broken Symmetry approach" by Francesco Cappelluti (2015).
- o Coadvisor of the PHD Thesis in Computational Chemistry "A theoretical approach to density-based molecular photochemistry for the study of remarkable properties relating to molecular excited states" by Federica Maschietto (2019).

## International Collaborations

- o Dr. Ilaria Ciofini (CNRS, Paris): Development and application of theoretical tools for the description of complex chemical phenomena.
- o Prof. Benedetta Mennucci (Università di Pisa, Italy): Simulation of Exciton Coupled Circular Dichroism spectra of biomolecules.
- o Prof. Barbara Kirchner (Mulliken Center, Bonn, Germany): Structure and Optical properties of Ionic Liquids.
- o Prof. Leonardo Guidoni (Università dell'Aquila, Italy): Quantum mechanical properties of biological objects (Vibrational (bio)spectroscopy).
- o Dr. Giacomo Prampolini (ICCOM-CNR, Pisa, Italy): Vibronically resolved UV/ECD through single-state and quantum dynamics approaches.
- o Prof. Enrico Bodo (Università di Roma La Sapienza, Italy): Material modeling by means ab-initio Molecular Dynamics and Classical Molecular Dynamics of Ionic Liquids.

## Articles

Coauthor of 36 publications on international journals, with 457 citations and h-index equal to 14 on Scopus (June 15th 2020). Author ID on Scopus: 35754430000. Asterisk indicates corresponding authorship (10). Among the 36 publications, 1 volume cover (article [7])

### Publications

- [1] L. Huet, A. Perfetto, F. Muniz-Miranda, M. Campetella, C. Adamo, and I. Ciofini, A general density-based index to analyze charge transfer phenomena: from models to butterfly molecules, *Journal of Chemical Theory and Computation*, vol. XXX, p. XXX, DOI: 10.1021/acs.jctc.0c00296 (2020).
- [2] (\*) M. Campetella, N. M. Nguyen, J. Baima, L. Maschio, F. Mauri, M. Calandra, Hybrid-functional electronic structure of multilayer graphene, *Physical Review B*, vol. 101, p. 165437, DOI: 10.1103/PhysRevB.101.165437 (2020).
- [3] (\*) M. Campetella, J. S. Garcia, Following the Evolution of Excited States along Photochemical Reaction Pathways, *The Journal of Computational Chemistry*, Vol. 41, p. 1156-1164, DOI: 10.1002/jcc.26162 (2020).
- [4] (\*) M. Campetella, F. Cappelluti, L. Gontrani, Medium Range Interactions Evidences in Compounds with Aliphatic Lateral Chain : 1-Pentanoic Acid, 1-Pentanol and Pentylammonium Nitrate

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- as Test Cases, *Chemical Physics Letters*, vol. 734, p. 136738, DOI: 10.1016/j.cplett.2019.136738 (2019).
- [5] F. Ramondo, L. Gontrani, M. Campetella, Coupled hydroxyl and ether functionalisation in EAH derivatives: The effect of hydrogen bond donor/acceptor groups on the structural heterogeneity studied with X-ray diffractions and fixed charge polarizable simulations, *Physical Chemistry Chemical Physics*, vol. 21, p. 11464-11475, DOI: 10.1039/C9CP00571D (2019).
- [6] J. S. Garcia, E. Bremond, M. Campetella, I. Ciofini, C. Adamo, Small Basis Set Allowing the Recovery of Dispersion Interactions with Double Hybrid Functionals, *Journal of Chemical Theory and Computation*, vol. 15, p. 2944-2953, DOI: 10.1021/acs.jctc.8b01293 (2019).
- [7] (\*) J. S. Garcia, M. Boggio-Pasqua, I. Ciofini, M. Campetella, Excited State Tracking During the Relaxation of Coordination Compounds, *The Journal of Computational Chemistry*, vol. 40, 1420-1428, DOI: 10.1002/jcc.25800 (2019).
- [8] (\*) M. Campetella, A. Perfetto, I. Ciofini, Quantifying partial hole-particle distance at the excited state: A revised version of the DCT index, *Chemical Physics Letters*, vol. 714, p. 81-86, DOI: 10.1016/j.cplett.2018.10.060 (2019).
- [9] F. Maschietto, J. Sanz Garcia, M. Campetella, I. Ciofini, Using density based indexes to characterize excited states evolution, *The Journal of Computational Chemistry*, vol. 40, p. 650-656, DOI: doi.org/10.1002/jcc.25750 (2018).
- [10] F. Maschietto, M. Campetella, M.J. Frisch, G. Scalmani, C. Adamo, I. Ciofini, How are the charge transfer descriptors affected by the quality of the underpinning electronic density?, *Journal of Computational Chemistry*, vol. 39, p. 735-742, DOI: 10.1002/jcc.25144 (2018).
- [11] (\*) M. Campetella, A. Mariani, C. Sadun, B. Wu, E.W. Castner Jr, L. Gontrani, Structure and dynamics of propylammonium nitrate-acetonitrile mixtures: An intricate multi-scale system probed with experimental and theoretical techniques, *The Journal of Chemical Physics*, vol. 149, p. 134507, DOI: 10.1063/1.5021868 (2018).
- [12] M. Campetella, A. Le Donne, M. Daniele, L. Gontrani, S. Lupi, E. Bodo, F. Leonelli, Hydrogen bonding features in cholinium-based protic ionic liquids from molecular dynamics simulations, *The Journal of Physical Chemistry B*, vol. 122, p. 2635-2645, DOI: 10.1021/acs.jpcc.7b12455 (2018).
- [13] J. Sanz Garcia, F. Maschietto, M. Campetella, I. Ciofini, Using Density Based Indexes and Wave Function Methods for the Description of Excited States: Excited State Proton Transfer Reactions as a Test Case, *The Journal of Physical Chemistry A*, vol. 122, p. 375-382, DOI: 10.1021/acs.jpca.7b10033 (2018).
- [14] M. Campetella, F. Maschietto, M.J. Frisch, G. Scalmani, I. Ciofini, C. Adamo, Charge transfer excitations in TDDFT: A ghost-hunter index, *Journal of Computational Chemistry*, vol. 38, p. 2151-2156, DOI: 10.1002/jcc.24862 (2017).
- [15] (\*) L. Gontrani, R. Caminiti, U. Salma, M. Campetella, A structural and theoretical study of the alkylammonium nitrates forefather: Liquid methylammonium nitrate, *Chemical Physics Letters*, vol. 684, p. 304-309, DOI: 10.1016/j.cplett.2017.07.017 (2017).

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- [16] O. Andreussi, I.G. Prandi, M. Campetella, G. Prampolini, B. Mennucci, Classical Force Fields Tailored for QM Applications: Is It Really a Feasible Strategy?, *Journal of Chemical Theory and Computation*, vol. 13, p. 4636-4648, DOI: 10.1021/acs.jctc.7b00777 (2017).
- [17] (\*) L. Gontrani, F. Leonelli, M. Campetella, An X-Ray and Computational Study of Liquid Pentylammonium Nitrate, *Chemical Physics Letters*, vol. 687, p. 38-43, DOI: 10.1016/j.cplett.2017.08.068 (2017).
- [18] (\*) M. Campetella, M. Macchiagodena, L. Gontrani, B. Kirchner, Effect of alkyl chain length in protic ionic liquids: an AIMD perspective, *Molecular Physics*, vol. 315, p. 1582-1589, DOI: 10.1080/00268976.2017.1308027 (2017).
- [19] M. Campetella, M. Montagna, L. Gontrani, E. Scarpellini, E. Bodo, Unexpected proton mobility in the bulk phase of cholinium-based ionic liquids: new insights from theoretical calculations, *Physical Chemistry Chemical Physics*, vol. 19, p. 11869-11880, DOI: 10.1039/C7CP01050H (2017).
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- [22] L. Cupellini, S. Jurinovich, M. Campetella, S. Caprasecca, C. A. Guido, S. M. Kelly, A. T. Cardiner, R. Cogdell, B. Mennucci, An ab initio description of the excitonic properties of LH2 and their temperature dependence, *The Journal of Physical Chemistry B*, vol. 120, p. 11348-11359, DOI: 10.1021/acs.jpcc.6b06585 (2016).
- [23] G. Prampolini, M. Campetella, N. De Mitri, P. R. Livotto, I. Cacelli, Systematic and automated development of quantum mechanically derived force fields: the challenging case of halogenated hydrocarbons, *Journal of Chemical Theory and Computation*, vol. 12, p. 5525-5540, DOI: 10.1021/acs.jctc.6b00705 (2016).
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- [25] M. Campetella, D. Bovi, R. Caminiti, L. Guidoni, L. Benvenuti, L. Gontrani, Structural and vibrational study of 2-methoxyethylammonium nitrate (2-omeean). Interpretation of experimental results with ab initio molecular dynamics, *The Journal of Chemical Physics*, vol. 145, p. 024507, DOI: 10.1063/1.4956459 (2016).
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- [34] M. Campetella, L. Gontrani, F. Leonelli, L. Bencivenni, R. Caminiti, Two different models to predict ionic-liquid diffraction patterns: Fixed-charge versus polarizable potentials, *ChemPhysChem*, vol. 16, p. 197-203, DOI: 10.1002/cphc.201402577 (2015).
- [35] M. Campetella, L. Gontrani, E. Bodo, F. Ceccacci, F. C. Marincola, R. Caminiti, Conformational isomerisms and nano-aggregation in substituted alkylammonium nitrates ionic liquids: An x-ray and computational study of 2-methoxyethylammonium nitrate, *The Journal of Chemical Physics*, vol. 138, p. 184506, DOI: 10.1063/1.4803799 (2013).
- [36] F. Ramondo, L. Tanzi, M. Campetella, L. Gontrani, G. Mancini, A. Pieretti, C. Sadun, Hydration of diazoles in water solution: pyrazole. a theoretical and x-ray diffraction study, *Physical Chemistry Chemical Physics*, vol. 11, p. 9431-9439, DOI: 10.1039/B909388E (2009).

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