ALLEGATO B

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[Marco Campetella]
CURRICULUM VITAE

INFORMAZIONI PERSONALI (NON INSERIRE INDIRIZZO PRIVATO E TELEFONO FISSO O CELLULARE)

COGNOME	CAMPETELLA
NOME	MARCO
DATA DI NASCITA	[26, 10, 1982]

INSERIRE IL PROPRIO CURRICULUM
(non eccedente le 30 pagine)

Personal Information

Date of Birth: 26 October 1982.
Place of Birth: Rome, Italy.

Appointments

Dr. Matteo Calandra's group, CNRS Paris
Postdoctoral Researcher September 2018–Ongoing
I'm characterizing both electronic and structural properties of different kinds of 2D materials. At the moment I'm focusing my attention on Bernal stacked bilayer graphene and the Misfit Layer Compound $LaNb_2La_5$.

Dr. Ilaria Ciofini's group, CNRS Paris
Postdoctoral Researcher September 2016–August 2018
I've characterized the excited states of different systems. I focused my attention on a series of push-pull molecules. In particular I'm analysing the behaviour of the D_{CT} parameter varying both the acceptor-donor distance and the functionals in the TDDFT calculations.

Prof. Benedetta Mennucci's group, Università di Pisa Pisa
Postdoctoral Researcher July 2015–July 2016
I have developed 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 lectures on quantum chemistry for PhD students.

University "La Sapienza" Rome
Assistant 2013–2014
During my PhD, I held the position of assistant for both the chemistry and the physics courses for the natural science bacherol degree.

Education

Università di Roma “La Sapienza”
Ph.D., Material Science October 2011–October 2014
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 di Roma “La Sapienza”
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 $La_{2-x}Sr_xCuO_4$ 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 study it was necessary the implementation of the mathematical model in a Fortran90 code, for
both the techniques.

Università di Roma “La Sapieza”
Bachelor’s Degree, Physics September 2006–September 2009
Università di Roma 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 perform 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 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 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 di Roma "La Sapienza"
Bachelor's Degree, Chemistry September 2001–September 2004

Fellowships

Università di Roma Roma
Graduate School "La Sapienza" Ph.D. Fellowship October 2011–October 2014

CINECA Roma
Graduate Fellowship, Material Science February 2008–July 2009
Topic: "Structural study in aqueous solution of heterocyclic systems such us 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.

Conferences & Schools

April 2018 Oral Presentation at the « ACS » (Boston, U.S.A.)
September 2017 European Summer School in Quantum Chemistry (Torre Normanna, Italy)
March 2017 Oral Presentation at the « TheoBio » (San Sebastian, Spain)
March 2017 Oral Presentation at the « CMS » (Warwick, U.K.)
April 2016 Oral Presentation at the « ACS » (San Diego, U.S.A.)
August 2015 CECAM 4th CP2K Tutorial
March 2013 Poster contribution at the « Winter Modeling » (Modena, Italy)
May 2012 CECAM Car-Parrinello Molecular Dynamics (CPMD) tutorial: understanding condensed matter and molecular physics

Computer skills

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

International Collaborations

Prof. Benedetta Mennucci (Università di Pisa, Italy): Simulation of Exciton Coupled Circular Dichroism spectra of biomolecules.
Prof. Barbara Kirchner (Mulliken Center, Bonn, Germany): Structure and Optical properties of Ionic Liquids.
Prof. Leonardo Guidoni (Università dell'Aquila, Italy): Quantum mechanical properties of biological objects (Vibrational (bio)spectroscopy).
Dr. Giacomo Prampolini (ICCOM–CNR, Pisa, Italy): Vibronically resolved UV/ECD through single-state and quantum dynamics approaches.
Prof. Enrico Bodo (University of Vigo, Spain): Material modeling by means ab-initio Molecular Dynamics and Classical Molecular Dynamics of Ionic Liquids.

Publications

[1] 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, DOI: 10.1021/acs.jctc.8b01203(2019).
[2] J. S. Garcia, M Boggio-Pasqua, I. Ciofini, M. Campetella, Excited State Tracking During the Relaxation of Coordination Compounds. The Journal of Computational Chemistry, DOI:10.1002/jcc.25800 (2019).
[3] 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 (2019).
[4] F. Maschietto, J. Sanz García, M. Campetella, I. Ciofini, Using density based indexes to characterize excited states evolution, The Journal of Computational Chemistry, vol. 40, p. 650-656 (2019).
[5] 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 (2018).
[6] 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 (2018).
[7] 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 (2018).
[8] J. Sanz García, 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 (2018).
[9] 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 (2017).
[10] 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 (2017).
[11] 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 (2017)
[12] L. Gontrani, F. Leonelli, M. Campetella, An X-Ray and Computational Study of Liquid Pentylammonium Nitrate, Chemical Physics Letters, vol. 687, p. 38-43 (2017).
[13] M. Campetella, M. Macchiagodena, L. Gontrani, B. Kirchner, Effect of alkyl chain length in protic ionic liquids: an AIMD perspective, Molecular Physics, vol. 115, p. 1582-1589 (2017).
[14] 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 (2017).
[15] L. Gontrani, E. Scarpellini, R. Caminiti, M. Campetella, Bio ionic liquids and water mixtures: a structural study, RSC Advances, vol. 7, p.19338-19344 (2017).
[16] A. Mariani, M. Campetella, C. Fasolato, M. Daniele, F. Capitani, L. Bencivenni, P. Postorino, S. Lupi, R. Caminiti, L. Gontrani, A joint experimental and computational study on ethylammonium nitrate-ethylene

glycol 1: 1 mixture. Structural, kinetic, dynamic and spectroscopic properties, Journal of Molecular Liquids, vol. 226, p. 2-8 (2017).
[17] L. Cupellini, S. Jurinovich, M. Campetella, S. Caprasecca, C. A. Guido, S. M. Kelly, A. T. Gardiner, 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 (2016).
[18] 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 (2016).
[19] M. Campetella, D. C. Martino, E. Scarpellini, L. Gontrani, Low-q peak in x-ray patterns of choline-phenylalanine and-homophenylalanine: A combined effect of chain and stacking, Chemical Physics Letters, vol. 660, p. 99-101 (2016).
[20] M. Campetella, D. Bovi, R. Caminiti, L. Guidoni, L. Bencivenni, 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 (2016).
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[22] M. Campetella, E. Bodo, M. Montagna, S. De Santis, L. Gontrani, Theoretical study of ionic liquids based on the cholinium cation. ab initio simulations of their condensed phases, The Journal of Chemical Physics vol. 144, p. 104504 (2016).
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[24] A. Mariani, R. Caminiti, M. Campetella, L. Gontrani, Pressure-induced mesoscopic disorder in protic ionic liquids: first computational study, Physical Chemistry Chemical Physics, vol. 18, p. 2297-2302 (2016).
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[26] M. Campetella, E. Bodo, R. Caminiti, A. Martino, F. DApuzzo, S. Lupi, L. Gontrani, Interaction and dynamics of ionic liquids based on choline and amino acid anions, The Journal of Chemical Physics, vol. 142, p. 234502 (2015).
[27] 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 (2015).
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