Curriculum Vitae

Giacomo Prampolini was born in La Spezia in 1973. He took his degree in Chemistry (in 2000, *cum laude*) at the University of Pisa under the supervision of Prof. Ivo Cacelli. In 2001, he attended the School of Graduate Studies G. Galilei in Pisa, obtaining his PhD degree in 2005 with a thesis titled "Computer Simulations With Quantum Mechanically Derived Force-Fields". Since 2005, GP has won a four-year Post-Doctoral fellowship at the University of Pisa and, in 2009, a Post-Doctoral fellowship at the Department of Chemistry "Paolo Corradini" of the University of Naples (titled "*In silico* design of biosensor based on nanostructured materials"). Between 2006 and 2008 GP has cooperated in the national research project (PRIN) titled "Theoretical models and methods for the computation and simulation of properties and dynamical processes in molecular and supra-molecular systems and in condensed phases". In 2010, GP won a Post-Doctoral fellowship at the Scuola Normale Superiore (SNS) in Pisa, titled "Time-dependent and time-independent approaches to computational spectroscopy". In November 2011 he obtained a Research Scientist position at the Institute of Physical and Chemical Procecesse (IPCF) of the National Research Council (CNR), he is currently working at the Institute for the Chemistry of Organo-Metallic Compounds (ICCOM). In the past three years, GP actively participated at two projects: the POLOPTEL project on smart materials, founded by the Fondazione Cassa di Risparmio di Pisa and the PRIN project titled "PROXY". Finally, he recently won a short-term visiting professor position within the CAPES project, founded by the Brazilian Ministry of Education. where is currently working

GP scientific interests focus on theoretical and computational physical chemistry. Since 2000, he worked with Prof. Ivo Cacelli (University of Pisa) on the implementation of novel strategies for force-fields parameterizations, suitable for computer simulations of condensed phases. In this field, GP has contributed to develop an original method for the computation of the intermolecular energy of large dimers

(Fragmentation Reconstruction Method, FRM) and to code the JOYCE software for parameterization of intra-molecular force fields from *ab initio* computed data. Since 2002 he has been working in the theoretical group of liquid crystals (TGLC) at the University of Pisa, focusing its work on computer simulations of liquid crystalline materials. Within this project, GP has studied dynamical and transport properties in condensed phases, with particular attention to sub-diffusive phenomena. More recently collaboration was started in this field with Prof. Paolo Roberto Livotto (Instituto do Quìmica, Universidade Federal do Rio Grande do Sul, Brazil). In 2008 he started to collaborate with Prof. Vincenzo Barone (SNS) and Dr. Alessandro Ferretti (ICCOM, CNR), participating in the development of novel computational methods for the accurate calculation of the magnetic splitting in di-radical compounds of potentially technological interest. In 2009 and 2011, two collaborations with Dr. Susanna Monti (ICCOM, CNR) were started within the projects "*In silico* design of biosensor based on nano-structured materials" and POLOPTEL. The first regarded a computational study of genetic chips, focusing on a single strand DNA biosensor, whereas the second was focused on the development of accurate computational protocols for the design and interpretation of smart functionalized polymers. In these years, within the post-doctoral fellowship at the SNS, GP has also worked to the extension of the parameterization tools to excited states, to assist a time-dependent route to computational spectroscopy. GP took part on several congresses and workshops and is coauthor of 60 scientific articles on international peer-reviewed journals and 1 book chapter, with more than 500 citations and an h-index of 14. Since 2000, he has contributed to the coding of several computational chemistry software as MCGBLJ (Monte Carlo program for computer simulations with hybrid and coarse grained potentials), SIRIUS (fitting software for intermolecular parameterizations), JOYCE (parameterization of intramolecular force-fields), POLAF (fitting software for the time evolution of pair correlation functions), GETTO (topology generator utility, suitable in force-field

parameterization).

List of Publications

1) Cacelli, S. Campanile, G. Prampolini and A. Tani, "Stability of the Nematic Phase of 4-*n*-pentyl -4'-cyanobiphenyl Studied by Computer Simulation Using an Hybrid Model" *J. Chem. Phys.* **117**, 448 (2002)
2) C. Amovilli, I. Cacelli, S. Campanile and G. Prampolini, "Calculation of the Intermolecular Energy of Large Molecules by a Fragmentation Scheme: Application to the 4-**n**-pentyl-4'-cyanobiphenyl (5CB) Dimer" *J. Chem. Phys.* **117**, 3003 (2002)
3) I. Cacelli, G. Cinacchi, C. Geloni, G. Prampolini and A. Tani, "Computer Simulation of *p*-Phenyls with Interaction Potentials from *ab initio* Calculations" *Mol. Cry. Liq. Cry.* **395**, 171 (2003)
4) I. Cacelli and G. Prampolini, "Torsional Barriers and Correlation between Dihedral in *p*-Polyphenyls" *J. Phys. Chem. A* **107**, 8665 (2003)
5) G. Cinacchi and G. Prampolini, "DFT Study of the Torsional Potential in Ethylbenzene and Ethoxy Benzene: The Smallest Prototypes of Alkyl– and Alkoxy – Aryl Mesogens" *J. Phys. Chem. A* **107**, 5228 (2003)
6) I. Cacelli, G. Cinacchi, G. Prampolini and A. Tani, "Modeling Benzene with Single-site Potentials from *ab initio* Calculations: A Step forward Hybrid Models of Complex Molecules" *J. Chem. Phys.* **120**, 3648 (2004)
7) I. Cacelli, G. Cinacchi, G. Prampolini and A. Tani, "Computer Simulation of Solid and Liquid Benzene with an Atomistic Interaction Potential Derived from *ab initio* Calculations" *J. Am. Chem. Soc.* **126**, 14278 (2004)
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10) M. Bizzarri, I. Cacelli, G. Prampolini and A. Tani, "Intermolecular Force Fields of Large Molecules by the Fragmentation Reconstruction Method (FRM): Application to a Nematic Liquid Crystal" *J. Phys. Chem. A* **108**, 10336 (2004)
11) I. Cacelli, G. Prampolini and A. Tani, "Atomistic Simulation of a Nematogen using a Force-Field Derived from quantum Chemical Calculations" *J. Phys. Chem. B*, **109**, 3531 (2005)
12) I. Cacelli and G. Prampolini, "DFT Conformational Study of Banana Shaped Mesogens" *Chem. Phys.,* **314**, 283 (2005)
13) G. Cinacchi and G. Prampolini, "DFT Study of the Conformational Space of Phenyl Benzoate, a Common Fragment in Many Mesogenic Molecules" *J. Phys. Chem. A*, **109**, 6290 (2005)
14) L. De Gaetani, G. Prampolini and A. Tani "Modeling a Liquid Crystal Dynamics by Atomistic Simulation with an Ab Initio Derived Force Field" *J. Phys. Chem B*, **110**, 2847 (2006)
15) G. Prampolini, "Parametrization and Validation of Coarse Grained Force-Fields Derived from *ab initio* Calculations" *J. Chem. Theory Comput.*, **2**, 556 (2006)
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