(Last update: August 9th 2013)

## PROF. MAURO STENER, CURRICULUM VITAE

Mauro Stener was born at Trieste (Italy) on 13th June 1967, he obtained the "Maturita' Scientifica" (Liceo Galileo Galilei – Trieste) in summer 1986 with score 60/60. Then he attended Chemistry course at University of Trieste, where he graduated *cum laude* in chemistry in March 1992 with a thesis supervised by Prof. N. Rahman. In 1995 he completed his PhD in Theoretical Chemistry at University of Trieste under the supervision of Prof. P. Decleva, with a dissertation on the application of the Density Functional Theory to excited states of atoms and molecules. In 1996 M. Stener spent one Postdoctoral year at the "Lehrstuhl für Theoretische Chemie" of the Technischen Universität München (Germany), within the project "Human Capital Mobility" (contract EU Projekt ERB-CHRX-CT 94-0532), under the supervision of Prof. Dr. Notker Rösch. During this period M. Stener performed a research activity on Relativistic Density Functional Theory applied to metal clusters. Starting from april 1998 up to November 2006 M. Stener has been Assistant Professor ("Ricercatore") of Physical Chemistry at University of Trieste, where he was involved in research activity of theoretical and computational chemistry, in particular in the development of new Density Functional methods and algorithms for the study of photoionization and photoabsorption in molecules and clusters, as well as in application of computational methods to problems of inorganic and cluster chemistry. Starting from December 2006 up to now, Mauro Stener is Associate Professor of Physical Chemistry at the University of Trieste. Prof. M. Stener is author of 131 papers in international ISI journals with referee, and gave 81 contributions (posters and talks) at conferences or institutions. The ANVUR bibliometrics parameters are: the mean productivity of the last 10 years (2003-2012) is 80 articles in ten years, 1815 citations (normalized per academic age (19 years) gives 95.5 average citations per year, hc index = 13, h index =24).

Prof. Stener is married with Paola and has one daughter (Arianna) and one son (Carlo), born in 2003 (twins).

The research interests of Professor Stener are essentially in two fields:

**1. Molecular Photoionization**

The theoretical description of the molecular photoionization process is still an open field in quantum chemistry: the unbound photoelectron wave-function cannot be described with conventional basis functions due to the specific boundary conditions it must obey. In this field Prof. Stener has contributed to the developed of new original methods based on finite basis sets of B-spline functions to treat molecular photoionization, employing the Density Functional Theory (DFT) and its Time Dependent extension (TDDFT) to treat the electronic structure problem. In particular an original non-iterative TDDFT algorithm has been proposed and implemented, which has been proven very efficient, accurate and numerically stable (Stener et al., JCP 122 (2005) 234301). The suite of developed computer codes has been proven useful to study theoretically and therefore rationalize recent experiments in various fields. The codes have been also parallelized with standard MPI libraries, recent application on large systems have demonstrated the efficiency of the parallelization up to 256 cpu. Some recent and more relevant examples are:

- The DFT studies of dichroism effects in the photoelectron angular distributions from chiral molecules, see for example a) Stener et al. JCP 120 (2004) 3284, b) Stranges et al. JCP 122 (2005) 244303, c) Catone et al. PRL 108 (2012) 083001.

- The TDDFT studies of accurate photoionization dynamics of various molecules, see for example a) Stener et al. JCP 124 (2006) 114306, b) Toffoli et al. PRA 73 (2006) 042704 c) Toffoli et al. JCP 124 (2006) 214313 d) Stener et al. 134 (2011) 174311.

- The DFT studies of fullerenes (Venuti et al. JCP 111 (1999) 4589) and organometallic compounds (Decleva et al. PRL 95 (2005) 263401)

- Prof. Stener implemented in the B-spline codes the calculation of the Molecular Frame - Photoelectron Angular Distribution (MF-PAD), as described in the single author paper Stener CPL 356 (2002) 153, this field has recently promoted intense collaboration with the experimental group of A. Yagishita, see for example a) J. Adachi et al. JPB 40 (2007) 29 b) Mizuno at el. PRL 110 (2013) 043001 c) Yamazaki et al. PRL 101 (2008) 043004 c)

**2. Metal clusters**

Prof. Stener has started to work in this field during his Post-doc stay in Munich, see for example JCP 106 (1997) 5189, the most cited paper of M. Stener (cited 222 times). In this field M. Stener implemented in the ADF code a simplified TDDFT method to treat core electron excitations (Stener et al. CPL 373 (2003) 115), this computational scheme has been proven very useful to study XANES profiles in bulk materials employing finite size cluster models (see for example JPCB 110 (2006) 9899) and has been extended to include spin-orbit coupling (Stener et al. CPL 416 (2005) 56). Recently the photoabsorption of large gold nanoclusters (almost 200 atoms) have been calculated (Stener et al. JPCC 111 (2007) 11862) as well as nanoalloys in collaboration with A. Fortunelli (CNR-IPCF Pisa) (G. Barcaro et al. JPCC 115 (2011) 24085).

**Teaching activity**

Prof. Stener has been involved in teaching activities since 2000, giving lectures for Chemistry undergraduate students at various levels, on Physical Chemistry, Quantum Chemistry and Organic Physical Chemistry. He also organized a couple of courses for post-graduate PhD students on DFT and response theory.

In particular the official courses for chemistry Laurea: “Chimica Fisica Organica” (from 2000 to 2006), “Chimica Fisica 4” (from 2006 to now), “Chimica Quantistica” (from 2005 to now), “Chimica Fisica Ambientale” (from 2004 to 2008) and “Chimica Fisica” (for Laurea in Scienze Ambientali) (from 2007 to 2012) were assigned by the Faculty to prof. Stener.

Prof. Stener has also been invited to give a series of lectures on TDDFT at the “First International Training School on NanoAlloys (ISNA)” (Pisa 20-26 May 2012) sponsored by COST Action MP0903 NANOALLOY.

Professor Stener has been the supervisor of seven Laurea Thesis, four of them have been carried within the European Master in Theoretical Chemistry and Computational Modelling (TCCM) in collaboration with Universities of Barcelona, Madrid and Gröningen. Professor Stener has been the supervisor of two PhD students.

**Managerial and organization experience**

Prof. Stener has been involved in various projects funded by the Italian MIUR (PRIN and FIRB projects) and has been the National Coordinator of a PRISMA project (Innovative Project on Material Science) sponsored by INSTM (Italian Interuniversity Consortium on material Science and Technology) during the years 2005-2006.

Prof Mauro Stener has been:

- Vice-Director of the Dipartimento di Scienze Chimiche of Trieste University of Trieste from November 2008 to November 2010.

- Representative of Trieste University in the Directive Board of consortium INSTM (Florence) from November 2009 up to now

- Elected in the Directive Board of the Theoretical and Computational Chemistry Division of the Italian Chemical Society from 2010 up to now

- Director of the PhD School of Chemical and Pharmaceutical Sciences and Technologies of the Trieste University from June 2012 up to now.

- International Member of the Jury d'Habilitation of the University of Paris-Sud 11 (January 2011)

- Opponent for the final discussion of the PhD Thesis at Stockholm University, two times, april 2011 and june 2012.

- referee of FIRB projects of MIUR (Italian Ministery of University and Research)

- referee of VQR review of MIUR (Italian Ministery of University and Research)

- referee for the Department Of Energy (DOE) of USA

- member of the Americal Physical Society (APS)

- member of the Institute of Physics (MIsntP) (UK)

- referee for the following scientific journals: J. Chem. Phys., J. Phys. Chem., Chem. Phys., Chem. Phys. Letters, PCCP, Theoretical Chem. Accounts, JACS, J. Phys. B.

**Funding**

1) Prof. Stener has been the National Coordinator of the project PRISMA INSTM 2004 "Studio dei fenomeni di fotoassorbimento di core e di valenza in materiali cristallini e nanostrutturati", Anno 2004 Prot. PC-31/2004"

2) Participant of PRIN 2010 "DESCARTES - Development of Energy-targeted Self-assembled supramolecular systems: a Convergent Approach through Resonant information Transfer between Experiments and Simulations"

3) Participant of PRIN 2008 "MODELLI TEORICI E STUDI COMPUTAZIONALI DI OSSERVABILI SPETTROSCOPICHE DI SISTEMI CONDENSATI "

4) participant of PRIN 2006 "Metodi computazionali per lo studio di proprietà strutturali e dinamiche di nanoparticelle in sospensioni colloidali "

5) Participant of PRIN 2004 "MODELLI TEORICI E ALGORITMI COMPUTAZIONALI PER LE OSSERVABILI SPETTROSCOPICHE E LE PROPRIETA' DI RISPOSTA MOLECOLARE "

6) Participant of PRIN 2000 " MODELLI TEORICI E ALGORITMI PER L'INTERPRETAZIONE DI OSSERVABILI SPETTROSCOPICHE "

7) Participant of PRIN 1998 " Sviluppo di algoritmi per l'interpretazione di osservabili spettroscopiche "

8) Prof Mauro Stener has been the coordinator of one ISCRA B project for computational resources at CINECA and involved as participant in other three ISCRA projects

9) Prof Mauro Stener has been the coordinator of one HPC Grant 2010 project for computational resources at CASPUR.

**National Collaborations**

1) with Alessandro Fortunelli (CNR-IPCF Pisa) on optical properties of metal clusters and nanoalloys

2) with Monica De Simone: gas phase beam-line of Elettra synchrotron on photoabsorption and photoemission of gas phase molecules

3) with Stefano Turchini and Daniele Catone: POLAR Circular Polarization beam-line of Elettra synchrotron, for the study of dichroism of photoelectron angular distributions from chiral molecules

**International collaborations**

1) Akira Yagishita (Photon Factory, Institute of Materials Structure Science, KEK, Tsukuba, Japan) on Molecular Frame Photoelectron Angular Distributions (MF-PAD)

2) Yi Luo (Theoretical Chemistry, Department of Biotechnology Royal Institute of Technology, Stockholm, Sweden) on metal L-edges XANES and vibronic coupling.

3) Ivan Powis (School of Chemistry, University of Nottingham, UK) on dichroism of photoelectron angular distributions from chiral molecules.

4) Tamar Seideman (Northwestern University, Evanston, USA) on Theory of Time-Resolved Photoelectron Imaging

5) David Holland (Daresbury Laboratory, Daresbury, UK) on molecular photoionization

6) Ria Broer (Theoretical Chemistry, Zernike Institute for Advanced Materials, Groningen, The Netherlands) on semiconductor quantum dots and plasmonic gold clusters.

**Invited lectures at international conferences:**

**1)** "Molecular Photoionization: a density functional approach with applications to circular dichroism in photoelectron angular distribution"

International Networking for Young Scientists: "Chirality in Molecular Physics"

British Council, Paris, France, 7-11 March 2005 (invited lecture)

**2)** "A TDDFT study on the dichroism in the photoelectron angular distribution from a chiral transition metal compound"

Gordon Research Conference: "Photoions, Photoionization & Photodetachment" January 31 - February 5, 2010, Hotel Galvez, Galveston (Texas - USA)

Invited lecture.

**3)** " The TDDFT approach for the description of core electron excitations in bulk materials and large clusters"

Actinet I3 Workshop: Coupling XAS and Theoretical Chemistry for Heavy Atoms. Avignon (F), 23-24 June 2010, invited lecture.

**4)** "TDDFT computational study of optical photoabsorption in $Au_n$ and $Au_nAg_m$ nanoclusters"

European Cost Action MP0903: "Nanoalloys as advanced materials: from structure to properties and applications" Joint Working Group Meetings, Faculty of Chemistry, Universitat de Barcelona, April 14-16, 2011, invited lecture.

**5)** "TDDFT and DFT approaches for core electron excitations: molecules, bulk materials and large clusters"

CECAM workshop on: "X-ray Spectroscopy : Recent Advances in Modelling and New Challenges" July 13, 2011 to July 15, 2011, CECAM-ETHZ, Zurich, Switzerland, invited lecture.

**6)** "Core electron excitations in molecules, large clusters and bulk materials: a TDDFT approach"

Workshop: "Holistic Computational Spectroscopy" CMST Action CM1002 CODECS: COnvergent Distributed Environment for Computational Spectroscopy,

Pisa, Scuola Normale Superiore, 16 – 18 novembre 2011, invited lecture.

**7)** "C1s and F1s photoelectron angular distribution from oriented CH3F molecules: a combined theoretical TDDFT and experimental study"

MPS2012, International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces, August 27 - September 1, 2012, Berlin (Germany), invited lecture.

**8)** "TDDFT computational study of optical photoabsorption in $Ag_nPt_m$ nanoclusters"

European Cost Action MP0903: "Nanoalloys as advanced materials: from structure to properties and applications" Workshop - Working groups 2 and 4, Domaine de Valpré, Lyon, France, 7 – 9 April 2013, invited lecture.