COMMUNICATIONS OF PROF. M. STENER

1) M. Stener, P. Decleva and A. Lisini, "Theoretical Studies of Photoexcitation and Photoionization by Xα Hartree-Fock-Slater Approach in Atoms and Molecules", NATO ASI on "Density Functional Theory", Il Ciocco, Castelvecchio Pascoli (Lucca), 15 - 27 agosto 1993.

2) M. Stener, P. Decleva and A. Lisini, "Theoretical Studies of Photoexcitation and Photoionization by X□ Hartree-Fock-Slater Approach in Atoms and Molecules", "5th International Conference On the Applications of the Density Functional Theory in Chemistry and Physics", Villa Olmo, Como 13-16 settembre 1993.

3) M.Stener, P. Decleva and A. Lisini, "Stieltjes Imaging photoionization cross sections by large basis set LCAO density functional calculation", II convegno nazionale di informatica chimica, CINECA, Casalecchio di Reno, Bologna, 16-18 febbraio 1994.

4) P. Decleva, A. Lisini, M. Stener and G. Fronzoni, "Theoretical Study of inner shell absorption spectra in transition metal compounds", Secondo convegno SILS (Societa' Italiana Luce di Sincrotrone), Universita' di Roma "Tor Vergata", Roma 20-21 giugno 1994.

5) M.Stener, P. Decleva and A. Lisini, "Stieltjes Imaging photoionization cross sections by large basis set LCAO density functional calculation", Secondo convegno SILS (Societa' Italiana Luce di Sincrotrone), Universita' di Roma "Tor Vergata", Roma 20-21 giugno 1994.

6) P. Decleva, A. Lisini, M. Stener and G. Fronzoni, " Theoretical Study of inner shell absorption spectra in transition metal compounds", Secondo convegno INCM (consorzio interuniversitario nazionale per la chimica dei materiali), Firenze 13-15 febbraio 1995.

7) M. Stener, P. Decleva and A. Lisini, " Cross sections calculations by the LDA and TDLDA approaches", ICES-6, 6th International Conference on Electron Spectroscopy, Roma 19-23 giugno 1995.

8) M. Stener, P. Decleva and A. Lisini, " Cross sections calculations by the LDA and TDLDA approaches", XVIII congresso nazionale societa' chimica italiana, Milano 28 agosto- 1 settembre 1995.

9) M. Stener, P. Decleva and A. Lisini, "Density functional and ab-initio calculations of core excitation spectra", "6th International Conference On the Applications of the Density Functional Theory in Chemistry and Physics", Parigi, 29 agosto - 1 settembre 1995.

10) M. Stener, P. Decleva and A. Lisini, "Density functional - time dependent local density approximation calculations of autoionization resonances in noble gases", "6th International Conference On the Applications of the Density Functional Theory in Chemistry and Physics", Parigi, 29 agosto - 1 settembre 1995.

11) O. D. Häberlen, S. C. Chung, M. Stener and N. Rösch, "Dai cluster allo stato solido. Studio di una serie di cluster di oro Au_n, n = 6 ... 147 con il metodo del funzionale densita' relativistico", "XXVIII Congresso Nazionale della Divisione di Chimica Fisica della Societa' Chimica Italiana", Pisa, 10 - 14 febbraio 1997.

12) M. Stener, G. De Alti, G. Fronzoni and P. Decleva, "TDLDA calculations of photoionization cross-section and asymmetry parametr profiles of alkaline-earth atoms", "7th International Conference On the Applications of the Density Functional Theory in Chemistry and Physics", Vienna, 2 - 6 settembre 1997.

13) P. Decleva and M. Stener, "Molecular photoionization cross-section profiles and asymmetry parameter from B-spline LDA calculations", "7th International Conference On the Applications of the Density Functional Theory in Chemistry and Physics", Vienna, 2 - 6 settembre 1997.

14) M. Stener, "Theoretical Methods of Molecular Photoionization", "Chemistry Meeting - Universities of Ljubljana, Trieste and Zagreb", Trieste, 1 - 2 luglio 1998.

15) M. Stener, M. Venuti e P. Decleva, "Calcolo di orbitali molecolari dello spettro continuo con un metodo funzionale densità in una base di B-splines", "XXIX Congresso Nazionale della Divisione di Chimica Fisica della Societa' Chimica Italiana", Comunicazione Orale, Taormina (ME), 5 - 9 ottobre 1998.

16) M. Stener, G. Fronzoni, S. Furlan and P. Decleva, "Photoionization by TD-DFT and exchange correlation potential with correct asymptotic behaviour", "8th International Conference On the Applications of the Density Functional Theory to Chemistry and Physics", Roma, 6 - 10 settembre 1999.

17) P. Decleva , G. Fronzoni, M. Stener and G. De Alti, "Photoionization of C_{60} and M@C_{60} by large scale LDA continuum calculations", "8th International Conference On the Applications of the Density Functional Theory to Chemistry and Physics", Roma, 6 - 10 settembre 1999.

18) G. Fronzoni, M. Stener and P. Decleva, "Studio teorico degli spettri NEXAFS Cl 1s e 2p di Cl_2, ClF e ClF_3", "XXV Congresso Internazionale dei Chimici Teorici di Espressione Latina", Napoli, 13 – 18 settembre 1999.

19) M. Stener, G. Fronzoni, S. Furlan and P. Decleva, "Photoionization by TD-DFT and exchange correlation potential with correct asymptotic behaviour", "XXX Congresso Nazionale della Divisione di Chimica Fisica della Societa' Chimica Italiana", Firenze, 26 settembre – 1 ottobre 1999.

20) P. Decleva , G. Fronzoni, M. Stener and G. De Alti, "Photoionization of C_{60} and M@C_{60} by large scale LDA continuum calculations", "XXX Congresso Nazionale della Divisione di Chimica Fisica della Societa' Chimica Italiana", Firenze, 26 settembre – 1 ottobre 1999.

21) M. Stener and P. Decleva, "Time – Dependent Density Functional calculations of molecular photoionization cross section: N_2 and PH_3", "Xth International Congress of Quantum Chemistry", Mentone (Francia) 5-10 giugno 2000.

22) P. Decleva, P. Colavita, G. Fronzoni and M. Stener, "DFT calculations of photoionization of C_{60} and M@C_{60}", "Xth International Congress of Quantum Chemistry", Mentone (Francia) 5-10 giugno 2000.

23) G. Fronzoni, M. Stener and P. Decleva , “Theoretical study of photoionization processes in organometallic compounds”, “XXXI Congresso Nazionale della Divisione di Chimica Fisica della Società Chimica Italiana”, Padova, 19-23 giugno 2001.

24) M. Stener, G. Fronzoni and P. Decleva, “Calculations of photoemission profiles of C_{60} and endohedral compounds”, “XXXI Congresso Nazionale della Divisione di Chimica Fisica della Società Chimica Italiana”, Padova, 19-23 giugno 2001.

25) G. Fronzoni, M. Stener and P. Decleva , “Theoretical study of photoionization processes in organometallic compounds”, “Thirteenth International Conference on Vacuum Ultraviolet Radiation Physics (VUV-XIII)”, Trieste, 23-27 luglio 2001.

26) M. Stener, G. Fronzoni and P. Decleva, “Calculations of photoemission profiles of C_{60} and endohedral compounds”, “Thirteenth International Conference on Vacuum Ultraviolet Radiation Physics (VUV-XIII)”, Trieste, 23-27 luglio 2001.

27) M. Stener, G. Fronzoni, and P. Decleva, ”Time Dependent Density Functional B-spline calculation of molecular photoionization”, "9th International Conference On the Applications of the Density Functional Theory to Chemistry and Physics", Madrid, 10 - 14 settembre 2001.

28) P. Decleva, G. Fronzoni, and M. Stener, “Valence and core photoemission in $M@C_{60}$ (M = Be, Mg, Ca)”, “19th International Conference on X-ray and Inner-Shell Processes”, Università di Roma “La Sapienza”, 24 – 28 giugno 2002.

29) M. Stener, G. Fronzoni, and P. Decleva, “Photoionization of oriented molecules: a time dependent density functional approach”, “19th International Conference on X-ray and Inner-Shell Processes”, Università di Roma “La Sapienza”, 24 – 28 giugno 2002.

30) M. Stener and G. Fronzoni, ”Time Dependent Density Functional B-spline calculation of molecular photoionization”, “Fourth Congress of the International Society for Theoretical Chemical Physics”, Marly-le-Roi (Parigi) , Francia, 9 – 16 luglio 2002.

31) G. Fronzoni and M. Stener, “TD-DFT calculations of core excitations in large systems”, “Fourth Congress of the International Society for Theoretical Chemical Physics”, Marly-le-Roi (Parigi) , Francia, 9 – 16 luglio 2002.

32) Corrado Crotti, Teresa Celestino, Erica Farnetti, Mauro Stener and Stefano Fontana, “Synchrotron radiation photoemission study of tungsten carbonyl complexes”, XXX Congresso Nazionale della Divisione di Chimica Inorganica della Societa’ Chimica Italiana, Modena 15 – 19 settembre 2002.

33) Tsustomu Watanabe and Mauro Stener, “Penning Ionization of Axial Symmetric Molecules by Optically Allowed Excited Atoms”, The Vth Asian International Seminar on Atomic and Molecular Physics, Nara-ken New Public Hall, Nara, Japan 2-5 October, 2002.

34) M. Stener, “Descrizione teorica della fotoemissione e del fotoassorbimento di atomi e molecole”, "incontro scientifico COFIN", Universita’ di Siena 25 – 26 ottobre 2002, comunicazione orale.

35) M. Stener, G. Fronzoni and P. Decleva, “Descrizione della fotoionizzazione molecolare a livello DFT con funzioni di base B-spline”, “XXI Congresso della Societa’ Chimica Italiana”, Torino, 22-27 giugno 2003.

36) J. Schiessling, M. Stener, L. Kjeldgaard, T. Balasubramanian, P. Decleva, J. Nordgren and P. A. Brühwiler, “Angular Effects in Photoelectron Spectra of Solid and Monolayer C_{60}”, ICESS-9 (International Conference on Electronic Spectroscopy and Structure), Uppsala (Svezia), 30 giugno – 4 luglio 2003.

37) M. Alagia, G. Contini, P. Decleva, G. Fronzoni, T. Prosperi, R. Richter, M. Stener, S. Stranges, S. Turchini and N. Zema, “Photoionization of chiral, radical and transient free molecules at ELETTRA”, ICESS-9 (International Conference on Electronic Spectroscopy and Structure), Uppsala (Svezia), 30 giugno – 4 luglio 2003.

38) M. Stener, G. Fronzoni and A. Reduce, “Studio TDDFT delle eccitazioni di core in modelli molecolari della solfito ossidasi ”, GICC2003, V Edizione del Congresso del Gruppo Italiano di Chimica Computazionale, Certosa di Pontignano, Siena, 18-19 dicembre 2003, comunicazione orale.

39) M. Stener, “Time dependent density functional theory of core electron excitations”, DEMOCRITOS INFORMAL SEMINAR, SISSA, Trieste, 12 febbraio 2004.

40) J. Schiessling, M. Stener , T. Balasubramanian , L. Kjeldgaard, P. Decleva, J. Nordgren and P. A. Brühwiler, “Identification of molecular orbital components of C60 on Al(110)”, “205th Meeting of The Electrochemical Society”, 9–14 May 2004, San Antonio, Texas, USA, comunicazione orale.

41) S. Turchini, N. Zema, G. Contini, G. Alberti, M. Alagia, S. Stranges, G. Fronzoni, M. Stener, P. Decleva and T. Prosperi
"Circular Dichroism in the Angular Distribution of Photoelectrons from Chiral Molecules: Experiment and Theory on R(+) and S(-) Methyl-oxiranes"
INFMEETING 2004, Convegno nazionale per la Ricerca Interdisciplinare in Fisica della materia (CNR-INFM), Genova 8-10 giugno 2004, poster.

42) M. Stener, R. De Francesco, G. Fronzoni
“Eccitazioni di core in ossidi metallici: studio TDDFT con modelli a cluster”
Divisione di Chimica Fisica - Società Chimica Italiana, XXXIII Congresso Nazionale, 21 - 25 Giugno 2004, Napoli - Complesso Universitario di Monte S. Angelo, poster.

43) M. Stener,

" Photoionization of large polyatomic molecules and clusters (Theory)"

3rd meeting of the COST working group D26/0002/02: "B-spline basis sets in laser-molecule interactions: ionisation and active control of chemical reactions", Università di Trieste, Italy, 1 and 2 October 2004, comunicazione orale.

44) M. Stener

"Density Functional Theory of Photoionization"

Nottingham University (England), 3 novembre 2004, seminario su invito.

45) M. Stener

"Quantum chemistry approaches to predict ion fragmentation in the gas phase", Shimadzu Research Laboratory (Europe)LTD., Manchester, England, 5 novembre 2004, seminario su invito.

46) M. Stener, R. De Francesco, G. Fronzoni

"Eccitazioni di core in ossidi metallici: studio TDDFT con modelli a cluster"

III Scuola Nazionale in Simulazioni Computazionali Multiscala Applicate alle Scienze dei Materiali, 14-18 febbraio 2005, Modena - Università di Modena e Reggio Emilia (poster)

47) M. Stener

"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 talk)

48) S. Coriani, P. Decleva, G. Fronzoni, M. Stener, R. De Francesco, D. Di Tommaso e D. Toffoli,

"Struttura elettronica e spettri di eccitazione di cluster finiti"

Workshop presentazione Centro Interdipartimentale per le Scienze Computazionali (CISC)

Universita' di Trieste, 15 giugno 2005 (talk)

49) M. Stener, G. Fronzoni and P. Decleva
"Time Dependent Density Functional Theory for molecular photoionization with non-iterative algorithm and multicenter B-spline basis set: implementation and applications",
"11th International Conference On the Applications of the Density Functional Theory to Chemistry and Physics", Geneve, 11 - 15 September 2005, (poster).

50) G. Fronzoni, R. De Francesco, M. Stener and M. Causà,
"Time Dependent Density Functional Theory of X-ray absorption spectroscopy of metal oxides",
"11th International Conference On the Applications of the Density Functional Theory to Chemistry and Physics", Geneve, 11 - 15 September 2005, (poster).

51) D. Di Tommaso, M. Stener and P. Decleva
" Calculation of the Circular Dichroism in the photoelectron Angular Distribution with the LCAO B-spline DFT method"
"11th International Conference On the Applications of the Density Functional Theory to Chemistry and Physics", Geneve, 11 - 15 September 2005, (poster).

52) M. Stener e G. Fronzoni
"Time Dependent DFT per lo studio di sistemi estesi" (talk)
Presentazione SeaSandS 19-20 dicembre 2005, Dip. di Chimica Università Federico II, Complesso Universitario Monte Sant'Angelo, Napoli.

53) G. Fronzoni, R. De Francesco, M. Stener and M. Causa'
"Time Dependent Density Functional Theory of X-ray absorption spectroscopy of metal oxides"
XIII Elettra Users' Meeting, Satellite Workshop "Computer Simulations of Surface and Interface Phenomena", Trieste, 15-16 December 2005 (poster)

54) G. Fronzoni, R. De Francesco, M. Stener and M. Causa'
"X-Ray absorption spectroscopy of alkaline-earth and transition metal oxides by Time Dependent Density Functional Theory"
DFTEM2006 - International Conference on Density Functional Theory (DFT) and Transmission Electron Microscopy (TEM), Vienna, April 21 - 23, 2006

55) G. Fronzoni, R. De Francesco e M. Stener
"Calcoli TDDFT di eccitazioni di core in ossidi metallici e molecole adsorbite su superfici"
GICC2006, VI Convegno nazionale del Gruppo Interdivisionale di Chimica Computazionale, Isola di San Servolo, Venezia 18-21 dicembre 2006 (comunicazione orale).

56) M. Stener, A. Nardelli, R. De Francesco and G. Fronzoni
"Valence electron excitations in gold clusters: a scalar relativistic TDDFT study"
GICC2006, VI Convegno nazionale del Gruppo Interdivisionale di Chimica Computazionale, Isola di San Servolo, Venezia 18-21 dicembre 2006 (poster).

57) M. Stener, M. Causà, R. De Francesco, G. Fronzoni, A. Nardelli
"Core and valence TDDFT studies on bulk, nanostructured materials and surface adsorbed molecules"
INSTM2007, VI Convegno nazionale sulla Scienza e tecnologia dei materiali, Universita' degli Studi di Perugia, Aula Magna, 12-15 Giugno 2007 (poster).

58) M. Stener
"Applications of TDDFT to material science: core electron excitations of bulk materials and optical spectra of gold nanoparticles"
NNL (National Nanotechnology Laboratories) of CNR-INFM, Universita' degli Studi di Lecce, 20 giugno 2007, seminario su invito.

59) T. Teramoto, J. Adachi, K. Hosaka, M. Yamazaki, K. Yamanouchi, N. A. Cherepkov, M. Stener, P. Decleva and A. Yagishita
"New approach for a complete experiment: C1s photoionization in CO_2 molecules"
XXV ICPEAC, Freiburg, 25-31 July 2007

60) A. Yagishita, T. Teramoto, J. Adachi, K. Hosaka, M. Yamazaki, K. Yamanouchi, N. Cherepkov, M. Stener, P. Decleva
"New approach for a complete experiment: C1s photoionization of CO_2 and CS_2 molecules"
XV VUV, Berlin, 29 July - 3 August 2007.

61) M. Stener, P. Decleva and G. Fronzoni
"Response effects in photoemission of transition metal compounds by TDDFT"
The first Meeting of the COST Ation CM0702: Chemistry with Ultrashort Pulses and Free-Electron Lasers: Looking for Control Strategies Through "Exact" Computations (CUSPFEL) Bordeaux (France) 16 - 17 October 2008.

62) M. Stener, G. Fronzoni, A. Nardelli and R. De Francesco
"Photoabsorption of gold nanoparticles: a TDDFT analysis by cluster model"
Theoretical Tools for In-silico Spectroscopy (TheTIS)
Pisa, 18-20 February 2009, Oral contribution

63) M. Stener, P. Decleva, M. Yamazaki, J. Adachi, T. Teramoto and A. Yagishita
"Photoelectron angular distribution from core ionization of a single oriented NO_2 molecule"
COST action CM0702, International Workshop on ATOMIC PHYSICS: "Ultra-fast dynamics in finite atomic and molecular systems probed with novel light sources",

Max Planck Institute for the Physics of Complex Systems (MPIPKS), Dresden, 23 - 25 november 2009, poster.

64) M. Stener
"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 talk.

65) M. Stener
"Resonances in chiral photoemission from a transition metal compound"
COST ACTION CM0702, 1st Meeting of the WG2, Universita' di Trieste, 22-24 April 2010, comunicazione orale.

66) D. Catone, S. Turchini, T. Prosperi, N. Zema, G. Contini, V. Feyer, M. Beccari, K. C. Prince, M. Stener, P. Decleva
"Gas phase circular dichroism in the photoelectron spectroscopy of dissymmetric metal-organic complex: Co(III)-tris-(acetylacetonate)."
XVIII Meeting of the Italian Society for Synchrotron Radiation (SILS 2010), 24-26 June 2010, Padova, Italy, poster.

67) M. Stener
" 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 talk.

68) D. Catone, S. Turchini, T. Prosperi, N. Zema, G. Contini, V. Feyer, M. Beccari, K. C. Prince, M. Stener, P. Decleva
"GAS PHASE CIRCULAR DICHROISM IN THE PHOTOELECTRON SPECTROSCOPY OF ASYMMETRIC METAL-ORGANIC COMPLEX: Co(III)-tris-(acetylacetonate)."
10th European Conference on Atom, Molecules and Photons (ECAMP 10), Salamanca, Spain, July 4-9, 2010, poster.

69) A. Kivimäki, L. Avaldi, P. Bolognesi, M. Coreno, P. O'Keeffe, V. Feyer, J. Alvarez Ruiz, M. Stankiewicz, M. Stener, G. Fronzoni, P. Decleva
"Photoabsorption, photoionization and photoelectron – Auger electron coincidence studies of the SF6 molecule at and above the S 2p edge"
37th International Conference on Vacuum Ultraviolet and X-ray Physics (VUVX2010), University of British Columbia, Vancouver, BC, Canada,11-16 July 2010, poster.

70) Mauro Stener, Nicola Durante and Alessandro Fortunelli
"TDDFT computational study of optical photoabsorption in Aun and AunAgm 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.

71) Mauro Stener
"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, keynote lecture.

72) R. De Francesco, M. Stener, G. Fronzoni
"X-Ray absorption spectroscopy at the $L_{2,3}$ edges of transition metal oxides by relativistic time dependent density functional calculations"
XXIV Congresso Nazionale della Societa' Chimica Italiana
Lecce, 11 – 16 September 2011, poster.

73) M. Romeo, R. De Francesco, M. Stener, G. Balducci, G. Fronzoni
"C K-edge NEXAFS Spectra of Model Systems for C_2H_4 on Si(100): a DFT Simulation"
XXIV Congresso Nazionale della Societa' Chimica Italiana
Lecce, 11 – 16 September 2011, poster.

74) R. De Francesco, G. Fronzoni, M. Stener
"Theoretical study of near edge x-ray absorption fine structure spectra of metal phtalocyanines at C and N Kedges"
XXIV Congresso Nazionale della Societa' Chimica Italiana
Lecce, 11 – 16 September 2011, poster.

75) Mauro Stener
"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 talk.

76) M. Stener , D. Catone, P. Decleva, G. Contini, N. Zema, T. Prosperi, V. Feyer, K. C. Prince, S. Turchini
"Resonant Circular Dichroism of Chiral Metal-Organic complex"
Primo Congresso Nazionale della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana, Pisa, Area della Ricerca del CNR, 22 - 23 febbraio 2012, poster.

77) M. Stener, Piero Decleva, Tomoya Mizuno, Jun-ichi Adachi, Misato Kazama, Hiroaki Yoshida, and Akira Yagishita
"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 talk.

78) M. Stener
"Recent advances in the theoretical description of photoelectron angular distribution"
Scuola Normale Superiore, Pisa, December, 20^{th} 2012
Invited seminar

79) M. Stener
"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 talk.

80) M. Stener
"Metal clusters: electronic structure and photoabsorption TDDFT calculations"
Scuola di Dottorato in Scienze Molecolari, Università degli Studi di Padova, May 2^{nd} 2013, invited seminar.

81) O. Baseggio and M. Stener
"A New Valence Photoabsorption TDDFT Algorithm for Large Systems"
15th International Conference on Density Functional Theory and its Applications, September 9 – 13, 2013, Durham, UK, poster