CURRICULUM VITAE et STUDIORUM
Daniele Toffoli, PhD

PERSONAL

Date and place of birth:	25th July 1974, Conegliano (TV), Italy.
Citizenship:	Italian.
Work Address:	Department of Chemistry, Middle East Technical University, 06531 Ankara, Turkey.
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EDUCATION

Ph. D. /Theoretical Chemistry, Università degli Studi di Trieste, Trieste, Italy, 18th March 2003. Dissertation: "*Development and application of DFT-based methods in atomic and molecular photoionization*" (Advisor: Prof. Piero Decleva), in English.

M. Sc. /Bio-inorganic Chemistry, *summa cum laude* (first class honors), Università degli Studi di Trieste, Trieste, Italy, 16th July 1999. Dissertation: "*Structural characterization of the Co-C and Co-S bonds in Cobalamins by diffraction with synchrotron radiation*" (Advisor: Prof. Lucio Randaccio), in Italian.

CAREER HISTORY

10/2013-ongoing: *Assoc. prof.*, Dept. of Chemistry, Middle East Technical University, Ankara (Turkey).
09/2008-10/2013: *Assist. prof.*, Dept. of Chemistry, Middle East Technical University, Ankara (Turkey).
09/2006-08/2008: *Post-doctoral research associate*, Dept. of Chemistry, University of Aarhus (Denmark).
05/2005-08/2006: *Post-doctoral research associate*, INFM Democritos, Italy.
02/2003-02/2005: *Post-doctoral research associate*, Dept. of Chemistry, Texas A&M University, USA.
06/2000-12/2002: *Research assistant*, Dip. Scienze Chimiche, Universitá di Trieste, Italy**.**
02/2000-05/2000: *Research assistant*, Dip. Scienze e Tecnologie Chimiche, Universitá di Udine, Italy**.**
09/1998-07/1999: *Research assistant***,** Dipartimento di Scienze Chimiche, Universitá di Trieste, Italy**.**

AWARDS

1) Habilitation to Associate professor awarded by the Italian ministry of Research and Education (MIUR), Jan. 2014.
2) Assistant professorship, Department Chemistry, University of Aarhus, DK, 2008 (declined).
3) Post-Doctoral research fellowship, Department Chemistry, University of Aarhus, DK, 2006-2008.
4) Post-doctoral fellowship granted by the Ministerio de Ciencia y Innovación of Spain, under the program: "Modalidad C: Estancias de jóvenes doctores extranjeros en universidades públicas y centros de investigación españoles", 2007-2008 (declined).
5) Research Fellowship of the Italian Research Council, CNR, Italy, 2005-2006.
6) Robert A. Welch Post-Doctoral fellowship, Houston, TX, US, 2003-2005.
7) PhD fellowship, Universitá degli Studi di Trieste, Italy, 2000-2003.
8) Research fellowship Universitá degli Studi di Udine, Italy, 2000 (declined).

TRAINING COURSES (Selected)

1) "IX Summer School on Parallel Processing", Cineca, Bologna (Italy), 11-22 September 2000.
2) "Summer School in Molecular Physics and Quantum Chemistry", Jesus College, Oxford (UK), 9-14 September 2001.
3) "Scuola Estiva di Chimica Computazionale 2002: Stati eccitati, spettroscopia e processi fotochimici", Dipartimento di Chimica e Chimica Industriale, Università degli Studi di Pisa (Italy), 25–31 August 2002.
4) "Winter School in Theoretical Chemistry 2005. Nanophotonics", Chemistry Department, University of Helsinki, Helsinki (FI), 7-9 December 2005.
5) Workshop on Theoretical Chemistry 2006. Mariapfarr, Salzburg, Österreich, 14-17 February 2006.
6) "Time-dependent density-functional theory and the theory of dispersion forces and weak chemical interaction", Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, March-April 2006.
7) "Quantum Mechanics, classical diffusion, computer simulations", Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, March-April 2006.

8) "The 9th Sostrup Summer School: quantum chemistry and molecular properties", June 25-July 7, 2006, Himmelbjergegnens Natur- og Idrætsefterskole, Ry, Denmark.
9) "The 18th Jyväskylä Summer School", August 06-22 2008, University of Jyväskylä, Finland.
10) "PhD School of the INT-network CORINF on Correlated Multielectron Dynamics in Intense Light Fields", 11-15 June 2012, Max-Planck-Institut für Physik komplexer Systeme Dresden, Germany.

LANGUAGES

Italian (native language), English (fluent written and spoken, TOEFL 108/120).

COMPUTATIONAL SKILLS

Operating systems: good knowledge of UNIX/LINUX, WINDOWS, and Mac-OS X.
Programming Languages: good knowledge of FORTRAN77-FORTAN90/95, C++.
Basic Knowledge of parallel processing (MPI and OpenMP).
Quantum-chemical software: ADF package, Gaussian09, MOLPRO, DALTON, GAMESS-US, ACESII, CFOUR, PWscf.
Developer of quantum mechanical software: MidasCpp (Prof. Ove Christiansen's lab, Aarhus University, DK), as well as software for the treatment of photoionization and electron-molecule collision processes developed in collaboration with Prof. Decleva (University of Trieste, Italy) and Prof. R. R. Lucchese (Texas A&M University, US).

TEACHING ACTIVITY

1) CHEM107: General Chemistry for Engineers (ECTS credits: 6.0), fall 2008, spring 2009, METU.
2) CHEM252: Physical Chemistry I (ECTS credits: 7.0), spring 2014, METU.
3) CHEM254: Physical Chemistry Laboratory I (ECTS credits: 6.0), spring 2014, METU.
4) CHEM257: Mathematics for Chemists (ECTS credits: 7.5), fall 2009, spring 2010, summer 2010, fall 2010, fall 2011, fall 2012, fall 2013, METU.
5) CHEM489:Computational Chemistry (ECTS credits: 7.5), spring 2009, spring 2010, METU (new class designed for undergrads in chemistry).
6) CHEM597: Advanced topics in Physical Chemistry (ECTS credits: 8.0), fall 2009, spring 2011, spring 2012, spring 2013, spring 2014, METU.
7) CHEM111: General Chemistry I (ECTS credits: 6.0), fall 2010, fall 2011, fall 2012, fall 2013, METU.
8) CHEM112: General Chemistry II (ECTS credits: 6.0), spring 2012, spring 2013, METU.
9) CHEM429, Simulation Techniques in Theoretical Chemistry (ECTS credits: 7.5), spring 2011, METU (new class designed for undergrads in chemistry).
10) Invited lecturer at the "Summer School on Modelling Nanostructures using Density Functional Theory", Izmir, Turkey, 10-21 August 2009.
11) Invited lecturer at the "International Winter School on Physics and Chemistry of Solids", Ankara, Turkey, 6-12 November 2011.
12) Tutor for Physical Chemistry II (20 hrs), fall 2001, Univ. Trieste.

RESEARCH LINES

Part of my research concerns the accurate description of radiation-matter interaction and electron-molecule scattering through the development of software implementing the state-of-the-art methodologies of quantum chemistry. These approaches range from density functional theory (and its time-dependent generalization) to more sophisticated *ab-initio* methods. My involvement in this field started during my graduate studies and has resulted in publications in high quality international journals, and in the establishment of close collaborations with experimental researchers in international laboratories, both in Europe, Japan, and the US. More recently I have developed a novel computational approach to the calculation of nondipole effects in molecular photoemission. The code has been applied to large molecular systems, such as C_{60} and camphor. I also developed a computational approach for the calculation of molecular multiphoton ionization cross sections and photoelectron angular distributions in collaboration with Prof. Piero Decleva, at the University of Trieste.

Another research area is molecular quantum dynamics. I am a contributor to the MidasCpp software, developed in the lab of Prof. Ove Christiansen. I made original contributions to the development of algorithms for efficient construction of potential energy surfaces and novel vibrational wave-function methods. Among the various contributions are iterative procedures for the construction of potential energy surfaces (PESs) and their parameterization, extrapolation procedures, the development of fast algorithms for vibrational wave function methods, and the exploration of alternative primitive basis functions. All these developments are of crucial importance for a realistic description of the physics of soft matter and its interaction with light sources. My current interest in the field is the use of general curvilinear coordinates, for a more accurate description of soft vibrational modes, which are not properly described with traditional rectilinear coordinates.

I recently started research in the field of theoretical heterogeneous catalysis. Among my current interests are the design of more efficient NO_x storage-reduction catalysts, for which we are currently exploring the use of alternative supporting materials such as TiO_2 (anatase), and the effect of doping of the storage material (BaO) with alkaline metals for reducing sulphur poisoning. Other ongoing projects are the study of the role of promoters in the water-gas-shift reaction, the use of carbides as possible new efficient catalysts, and the study of the mechanism of the partial oxidation of alcohols on gold and silver catalysts. All these projects are carried out by using plane-wave DFT with open-source and commercial software such as PWscf and VASP.

STUDENTS SUPERVISION

1) Rukan Koşak (spring 2009, undergraduate project).
2) Ruslan Hummatov (co-advisor, MSc 2010, now PhD student at the University of New Mexico, US).
3) Mehmet Kiliç (spring 2011, undergraduate project).
4) Zuleyha Artuç (Principal advisor, MSc 2011).
5) Rukan Koşak (Principal advisor, MSc 2011, now PhD student at the Technische Universität Wien).
6) Mehmet Gokhan Sensoy (PhD thesis co-advisor, 2012-ongoing).
7) Mustafa Tek (PhD thesis co-advisor, 2012-ongoing).
8) Seda Kibar (PhD thesis principal advisor, 2012-ongoing).
9) Tugce Irfan-Ersoz (PhD thesis principal advisor, 2012-ongoing).
10) Merve Demirtas (PhD thesis co-advisor, 2012-ongoing).
11) Selma Bas (postdoc, 2012-ongoing).

NATIONAL AND INTERNATIONAL GRANTS FUNDED:

1) Bilateral TUBITAK (Turkish Council of Scientific and Technological Research)/CNR (Italy) Grant No. 209T083: "*Calculation of molecular multiphoton ionization cross sections*", (PI, 2010-2012).
2) Start-up from METU (BAP-01-03-2009-101) "*Development of new algorithms for Molecular quantum dynamics, electron-molecule scattering and molecular photoionization*", (PI, 2009-2011).
3) TUBITAK Grant No. 108T706: "*Density functional theory investigation of NO_x storage/reduction catalysts*". (Co-PI, 2009-2012).
4) TUBITAK Grant No. 112T542: "*Density Functional Theory design of highly active catalysts for clean H_2 production for fuel-cell applications*", (PI, 2012-2014).
5) TUBITAK Grant No. 113F099: "*Density Functional Theory investigation of the reaction mechanisms for selective oxidation of alcohols on gold catalysts*", (Co-PI, 2013-2016).
6) Bilateral TUBITAK/CNR Grant No. 113F377: "*Theoretical description of many-electron processes in photoionization*", (PI, 2014-2016).
7) TUBITAK "*The preparation, characterization, and investigation of H_2 uptake capacities of boron-based metal-organic frameworks*". (Co-PI, 2014-2016, **under review**).

PUBLICATIONS LIST

1) L. Randaccio, M. Furlan, S. Geremia, M. Slouf, I. Srnova and D. Toffoli, "Similarities and Differences between Cobalamines and Cobaloximes. Accurate Structural Determination of Methylcobalamin and of LiCl and KCl containing Cyanocobalamins by Sychtrontron Radiation", Inorganic Chemistry **39**(15), 3403-3413, 2000.
2) Lucio Randaccio, Silvano Geremia, Mauro Stener, Daniele Toffoli and Ennio Zangrando, "Electronic Properties of the axial Co-C and Co-S bonds in B-12 systems: a density functional study", European Journal of Inorganic Chemistry (1), 93-103, 2002.
3) D. Toffoli, M. Stener, G. Fronzoni and P. Decleva, "Convergence of the multicenter B-spline DFT approach for the continuum", Chemical Physics **276**(1), 25-43, 2002.
4) D. Toffoli, M. Stener, and P. Decleva "Application of the Relativistic Time Dependent Density Functional Theory to the photoionization of Xenon", Journal of Physics B: Atomic, Molecular and Optical Physics **35**(5), 1275-1305, 2002.
5) M. Stener, G. Fronzoni, D. Toffoli, P. Colavita, S. Furlan and P. Decleva , "Valence and core photoemission in M@C_{60} (M = Be, Mg, Ca)", Journal of Physics B: Atomic, Molecular and Optical Physics **35**(6), 1421-1438, 2002
6) D. Toffoli, M. Stener and P. Decleva, "Photoionization of Mercury: a Relativistic Time-Dependent Density-Functional-Theory Approach", Physical Review A **66**(1), Art. No 012501 (16 pages), 2002.
7) M Stener, G. Fronzoni, D. Toffoli and P. Decleva "Time dependent Density Functional Photoionization of CH_4, NH_3, H_2O and HF", Chemical Physics **282**(3), 337-351, 2002
8) D. Toffoli and P. Decleva , "Least Squares B-spline solutions of the radial Dirac equation in the continuum", Computer Physics Communications **152**(2), 151-164, 2003.
9) D. Toffoli, M. Stener, and P. Decleva, "3d photoionization along the Xenon isoelectronic sequence", Journal of Physics B: Atomic, Molecular and Optical Physics **36**(14), 3097-3118, 2003.
10) Daniele Toffoli and Robert R. Lucchese, "Near Threshold Photoionization of the ground and first excited state of C_2", The Journal of Chemical Physics **120**(13), 6010-6018, 2004.
11) Daniele Toffoli, Mary J. Simpson and Robert R. Lucchese "Cross-Section and Asymmetry-Parameter Calculations for the Outer- and Inner-Valence Photoionization of Ethane", Physical Review A **69**(6), Art. No 062712 (9 pages), 2004.
12) N. Saito, D. Toffoli, R. R. Lucchese, M. Nagoshi, A. De Fanis, Y. Tamenori, M. Oura, H. Yamaoka, M. Kitajima, H. Tanaka, U. Hergenhahn and K. Ueda "Symmetry- and multiplet-resolved N 1s photoionization cross sections of the NO_2 molecule", Physical Review A **70**(6), Art. No 062724 (9 pages), 2004 .
13) G. J. Rathbone, E. D. Poliakoff, John D. Bozek, Daniele Toffoli, and Robert R. Lucchese, "Photoelectron trapping in N_2O $7\sigma \rightarrow k\sigma$ resonant ionization", The Journal of Chemical Physics **123**(1), Art. No 014307 (9 pages), 2005.
14) M. Stener, D. Toffoli, G. Fronzoni and P. Decleva, "Time-Dependent Density Functional Study of the Photoionization Dynamics of SF_6", The Journal of Chemical Physics **124**(11), Art. No 114306 (13 pages), 2006.
15) D. Toffoli, M. Stener and P. Decleva, "Photoabsorption and Photoionization Dynamics Study of Silicon Tetrafluoride in the Framework of Time-Dependent Density Functional Theory", Physical Review A **73**(4), Art. No 042704 (14 pages), 2006.
16) D. Toffoli, M. Stener G. Fronzoni and P. Decleva, "Photoionization Cross Section and Angular Distribution Calculations of Carbon Tetrafluoride", The Journal of Chemical Physics **124**(21), Art. No 214313 (10 pages), 2006.
17) D. Toffoli, and P. Decleva, "Photoelectron Angular Distributions Beyond the Dipole Approximation. A Computational Study on the N_2 Molecule", Journal of Physics B: Atomic, Molecular and Optical Physics **39**(12), 2681-2691, 2006. (Appeared in IOP Select 2006 and Highlights of J. Phys. B 2006)
18) R. De Francesco, M. Stener, M. Causà, D. Toffoli and G. Fronzoni, "Time Dependent Density Functional investigation of the near-edge absorption spectra of V_2O_5", Physical Chemistry Chemical Physics **8**(37), 4300-4310, 2006.
19) Daniele Toffoli, Robert R. Lucchese, M. Lebech, J. C. Houver, and D. Dowek, "Molecular frame and recoil frame photoelectron angular distributions from dissociative photoionization of NO_2", The Journal of Chemical Physics **126**(5), Art. No 054307 (12 pages), 2007.
20) M. Stener, D. Toffoli, G. Fronzoni, and P. Decleva "Recent Advances in Molecular Photoionization by Density Functional Theory based Approaches", Theoretical Chemistry Accounts **117**(5-6), 943-956, 2007.

21) N. Berrah, R.C. Bilodeau, J.D. Bozek, I. Dumitriu, D. Toffoli and R. R. Lucchese, "Shape Resonances in K-shell Photodetachment of Small Size-Selected Clusters: Experiment and Theory", Physical Review A **76**(4), Art. No 042709 (6 pages), 2007.
22) D. Toffoli, J. Kongsted and O. Christiansen, "Automatic generation of potential energy and properties surfaces of polyatomic molecules in normal coordinates", The Journal of Chemical Physics **127**(20), Art. No 204106 (14 pages), 2007. (Also appeared on the December 1, 2007 issue of the Virtual Journal of Biological Physics Research)
23) H. Farrokhpour, M. Alagia, L. Avaldi, M. Bamdad, M. Coreno, P. Decleva, M. de Simone, R. Richter, S. Stranges, M Tabrizchi, and D. Toffoli, "Spin-orbit activated interchannel coupling in the 3d photoionization of barium atoms", Journal of Physics B: Atomic, Molecular and Optical Physics. **40**(20), 4005-4012, 2007.
24) D. Toffoli, P. Decleva, F. A. Gianturco, and R. R. Lucchese, "Density Functional Theory for the Photoionization Dynamics of Uracil", The Journal of Chemical Physics **127**(23), Art. No 234317 (8 pages), 2007. (Also appeared on the January 1, 2008 issue of the Virtual Journal of Biological Physics Research)
25) D. Toffoli, and P. Decleva, "A Multicentric Approach to the Calculation of Nondipolar Effects in Molecular Photoemission", The Journal of Chemical Physics **128**(23), Art. No 234101 (13 pages), 2008.
26) Mikkel Bo Hansen, Ove Christiansen, Daniele Toffoli, and, Jacob Kongsted, "A virtual vibrational self-consistent-field method for efficient calculation of molecular vibrational partition functions and thermal effects on molecular properties", The Journal of Chemical Physics **128**(17) Art. No 174106 (14 pages), 2008.
27) Mikkel Bo Hansen, Jacob Kongsted, Daniele Toffoli, and Ove Christiansen, "Vibrational Contributions to Indirect Spin-spin Coupling Constants Calculated via Variational Anharmonic Approaches", The Journal of Physical Chemistry A, **112**(36) 8436-8445, 2008.
28) P. Bolognesi, D. Toffoli, P. Decleva, V. Feyer, R. Flammini, L. Pravica, and L. Avaldi, "The dipole and non dipole parameters of the N K shell of the N_2 molecule up to 80 eV above threshold", Journal of Physics B: Atomic, Molecular and Optical Physics **41** Art. No. 221002, 2008 (Fast Track Communication, 5 pages) (Appeared in IOP Select 2008).
29) D. Toffoli, and P. Decleva, "Nondipolar Effects in the Photoionization Dynamics of Carbon Tetrafluoride", Physical Review A **78**(6), Art. No 063402, 2008 (10 pages).
30) M. Sparta, D. Toffoli, and O. Christiansen, "An Adaptive Density-Guided Approach for the generation of potential energy surfaces of polyatomic molecules", Theoretical Chemistry Accounts **123**(5-6), 413-429, 2009.
31) Eduard Matito, Daniele Toffoli, and Ove Christiansen, "A hierarchy of potential energy surfaces constructed from energies and energy derivatives calculated on grids", The Journal of Chemical Physics, **130**(13) Art. No 134104 (13 pages), 2009. (9^{th} most downloaded paper of the month, April 2009)
32) Manuel Sparta, Ida-Marie Høyvik, Daniele Toffoli, and Ove Christiansen, "Potential Energy Surfaces for Vibrational Structure Calculations from a Multiresolution Adaptive Density-Guided Approach: Implementation and Test Calculations", The Journal of Physical Chemistry A, **113**(30) 8712-8723, 2009.
33) Mikkel Bo Hansen, Manuel Sparta, Peter Seidler, Daniele Toffoli, and Ove Christiansen "A new formulation and implementation of vibrational self-consistent field (VSCF) theory", Journal of Chemical Theory and Computation, **6**(1) 235-248, 2010.
34) Daniele Toffoli, Manuel Sparta, and Ove Christiansen, "Accurate multimode vibrational calculations with a B-spline basis: Theory, Tests and an application to dioxirane and diazirinone", Molecular Physics, **109**(5) 673-685, 2011.
35) Daniele Toffoli and Piero Decleva, "Large Oscillations in the nondipolar asymmetry parameters from C_{60}", Physical Review A, **81**, 061201(R) (4 pages), 2010.
36) Manuel Sparta, Mikkel Bo Hansen, Eduard Matito, Daniele Toffoli, and Ove Christiansen, "Using energy derivativatives information in automated potential and surface construction and vibrational calculations", Journal of Chemical Theory and Computation, **6**(10) 3162-3175, 2010.
37) Peter Seidler, Mikkel Bo Hansen, Werner Gyorffy, Daniele Toffoli, and Ove Christiansen "Vibrational absorption spectra calculated from vibrational configuration interaction response theory using the Lanczos method", The Journal of Chemical Physics, **132**(16) Art. No 164105 (15 pages), 2010.
38) N. Berrah, R. C. Bilodeau, I. Dumitriu, D. Toffoli and R. R. Lucchese, "Shape and Feshbach Resonances in Inner-Shell Photodetachment of Negative Ions", Journal of Electron Spectroscopy and Related Phenomena, **183**(1-3) 64-69, 2011.
39) S. Korica, A. Reinköster, M. Braune, J. Viefhaus, D. Rolles, B. Langer, G. Fronzoni, D. Toffoli, M. Stener, P. Decleva, O. M. Al-Dossary, and U. Becker, "Partial Photoionization Cross section of C_{60} and C_{70}: A gas versus adsorbed phase comparison" , Surface Science, **604**(21-22) 1940-1944, 2010.

40) Daniele Toffoli, Manuel Sparta, and Ove Christiansen, "Vibrational spectroscopy of hydrogen-bonded systems: six-dimensional simulation of the IR spectrum of F-(H_2O) complex", Chemical Physics Letters, **510**(1-3) 36-41, 2011.
41) S. Stranges, M. Alagia, P. Decleva, M. Stener, G. Fronzoni, D. Toffoli, M. Speranza, D. Catone, S. Turchini, T. Prosperi, N. Zema, G. Contini, and Y. Keheyan, "The valence electronic structure and conformational flexibility of Epichlorohydrin", Physical Chemistry Chemical Physics, **13**(27) 12517-12528, 2011 (Also appeared in 2010-2011 *ELETTRA HIGHLIGHTS*).
42) Daniele Toffoli, Mauro Stener, Giovanna Fronzoni, and Piero Decleva, "Computational characterization of the HOMO-2 photoemission intensity oscillations in C-60", Chemical Physics Letters, **516**(4-6) 154-157, 2011.
43) R. Hummatov, O. Gulseren, E. Ozensoy, D. Toffoli, and H. Ustunel, "First-Principles investigation of NOx and SOx adsorption on Anatase-supported BaO and Pt overlayers", Journal of Physical Chemistry C, **116**(10) 6191-6199, 2012.
44) H. Toffoli, S. Erkoc, D. Toffoli, "Modeling of Nanostructures", in J. Leszczynski Ed. "Handbook of Computational Chemistry", Springer Science+Business Media B.V. 2012. Ch. 27, pp: 995-1041. (Invited chapter).
45) Daniele Toffoli, and Piero Decleva, "Density Functional Theory for Molecular Multiphoton Ionization in the Perturbative Regime", The Journal of Chemical Physics, **137**(13) Art. No 134103 (10 pages), 2012.
46) Daniele Toffoli, and Piero Decleva, "Multiphoton Core Ionization Dynamics of Polyatomic Molecules", Journal of Physics B: Atomic, Molecular and Optical Physics **46** Art. No. 145101, 2013 (9 pages) (Appeared in Highlights of Journal of Physics B 2013).
47) Eugene Kamarchik, Daniele Toffoli, Ove Christiansen, Joel M. Bowman, "Ab initio potential energy and dipole moment surfaces of the F−(H_2O) complex", Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, **119**, 59-62, 2014.
48) A. Nurioglu, H. Akpinar, F. Ekiz Kanik, D. Toffoli, L. Toppare, "Further Investigation of Intramolecular H-Bonding in Benzimidazole and EDOT Containing Monomer", Journal of Electroanalytical Chemistry, **693**, 23-27, 2013.
49) Serim Ilday, Hande Ustunel, F Ömer Ilday, Daniele Toffoli, Gizem Nogay, David Friedrich, René Hübner, Bernd Schmidt, Karl-Heinz Heinig, Rasit Turan, "Si nano-VINe: Electrical Percolation in Quantum-Confined nc-Si: SiO_2 Systems", *submitted*.
50) Muzaffer Özcan, Daniele Toffoli, Hande Ustunel, and Ilyas Dehri, "Insights into Surface-Adsorbate Interactions in Corrosion Inhibition Processes at the Molecular Level", Corrosion Science, **80**, 482-486, 2014.
51) Mehmet Koc, Sezin Galioglu, Daniele Toffoli, Hande Ustunel, Burcu Akata, "Effect of Ion-exchange on Structural, Electronic, and Vibrational Properties of the -O-Ti-O-Ti-O- Quantum Wires in ETS-10", *submitted to MRS proceedings*.
52) Andrea Gnoli, Hande Ustunel, Daniele Toffoli, Liyang Yu, Daniele Catone, Silvano Lizzit, Rosanna Larciprete, "Triisopropylsilyethynyl-pentacene in the gas phase and adsorbed on Au(111)", *submitted*.
53) Mehmet Koc, Sezin Galioglu, Daniele Toffoli, Hande Ustunel, Burcu Akata, "Understanding the Effects of Ion-Exchange in titanosilicate ETS-10: A Joint Theoretical and Experimental Study", *submitted*.
54) Eda Rende, Cihan Efe Kilic, Yasemin Udum, Daniele Toffoli, Levent Toppare "Electrochromic properties of multicolored novel polymer synthesized via combination of benzotriazole and N-functionalized 2,5-di(2-thienyl)-1H-pyrrole units", *submitted*.
55) Zuleyha Artuc, Hande Ustunel, and Daniele Toffoli, "First principles investigation of NO_2 and SO_2 adsorption on γ-Al_2O_3 supported mono- and diatomic metal clusters", *submitted*.

* corresponding author. Citations in total: 550+ (source: ISI web of science, 21/10/2013), *H-index*: 14.

ORAL COMMUNICATIONS AND POSTERS IN NATIONAL AND INTERNATIONAL CONFERENCES

1) L. Randaccio, S. Geremia, M. Slouf, I. Srnova, D. Toffoli, "Similarities and differences between cobalamins (B_{12} system) and their simple model cobaloximes", 34th International Conference on Coordination Chemistry, Edinburgh (England), 9-14 July 2000 (talk).
2) L. Randaccio, S. Geremia, G. Nardin, G. Tauzher, D. Toffoli, "Accurate X-ray structure of Vitamin B_{12} and of the two B_{12} cofactors by sinchrotron radiation data. Comparison with the simple cobaloxime model", 5th European Symposium on Vitamin B_{12} and B_{12}-Proteins Marburg (Germany), 10-15 September 2000 (talk).
3) D. Toffoli, "Fotoionizzazione atomica con algoritmo TDLDA relativistico", Riunione scientifica Programma di Ricerche Cofinanziate MURST 2000-2002, Roma 27 June 2001 (talk).
4) D. Toffoli, "Fotoionizzazione atomica con algoritmo TDLDA relativistico", 1° Sigma Aldrich Young Chemists Symposium, Riccione 18-19 October 2001 (poster).
5) D. Toffoli, "Atomic photoionization with a relativistic TD-DFT algorithm", Summer school in Molecular Physics and Quantum Chemistry, Jesus College, Oxford (UK), 9-14 September 2001 (poster).
6) P. Decleva, G. Fronzoni, M. Stener, and D. Toffoli, "Progress in LDA and TDLDA calculations of molecular photoionization", Italian-Swedish Workshop in Spectroscopy with Synchrotron Radiation: Experiment and Theory, Stockholm, Sweden, 7-8 December 2001 (talk).
7) M. J. Simpson, D. Toffoli, and R.R. Lucchese, "Outer and Inner Valence Photoionization Study of the Ethane Molecule", XX Southwest Theoretical Chemistry Conference, Texas Tech University, Lubbock, TX, USA, 13-15 November 2003 (poster).
8) D. Toffoli, and R.R. Lucchese, "Photo ionization of the Ground and First Excited State of C_2", XX Southwest Theoretical Chemistry Conference, Texas Tech University, Lubbock, TX, USA 13-15 November 2003 (poster).
9) D. Toffoli, "Application of the Schwinger Variational Method to Molecular Photoionization" XXI Southwest Theoretical Chemistry Conference, Galveston, TX, USA 22-23 October 2004 (talk).
10) D. Toffoli, "Theoretical Studies of Electron-Molecule Scattering and Molecular Photoionization" EPIC-EIPAM Conference, S. Martino al Cimino (Viterbo), Italy, 25-30 June 2005 (invited talk).
11) D. Toffoli, "Molecular Photoionization Dynamics Study with a Time Dependent DFT Approach", Department of Chemistry, University of Helsinki, Finland, 7-9 December 2005 (poster).
12) D. Toffoli, "Molecular Photoionization Dynamics in a DFT Framework", Meccanica Quantistica Molecolare: Metodi di Calcolo e Analisi di Nuovi Fenomeni. Incontro annuale delle unita' di ricerca, CASPUR, Rome, 20-21 January 2006 (talk).
13) D. Toffoli, "Nondipolar effects in molecular photoemission", 5th meeting of the COST working group D26/0002/02, B-spline basis sets in laser-molecule interactions: ionisation and active control of chemical reactions, Universidad Autónoma de Madrid, 27-28 October 2006 (invited talk).
14) H. Farrokhpour, M. Tabrizchi, M. Alagia, L. Avaldi, M. Bamdad, M. Coreno, P. Decleva, M. de Simone, R. Richter, S. Stranges, D. Toffoli, "Spin-Orbit Activated Interchannel Coupling in the 3d Photoionization of Barium Atoms", the Sixth SESAME User's Meeting, Amman, Jordan 17-19 November, 2007.
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