CURRICULUM VITAE ET STUDIORUM

Dr. Daniele Toffoli

PERSONAL

Date and place of birth:	25th of July1974, Conegliano (TV), Italia
Citizenship:	Italian
Work address:	Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli studi di Trieste
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EDUCATION

A. ACADEMIC DEGREES

PhD in Chemistry (theoretical chemistry), Università degli Studi di Trieste, 18th of March 2003.
MSc in chemistry (*summa cum laude*), Università degli Studi di Trieste, 16th of July 1999.

B. PARTICIPATION TO SCHOOLS/WORKSHOPS (SELECTION)

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 interactions", 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", 25 June-7 July 2006, Himmelbjergegnens Natur- og Idrætsefterskole, Ry, Denmark.
9) "The 18th Jyväskylä Summer School", 6-22 August 2008, University of Jyväskylä, Finland.
10) "PhD School of the ITN-network CORINF on Correlated Multielectron Dynamics in Intense Light Fields", 11-15 June 2012, Max-Planck-Institut für Physik komplexer Systeme Dresden, Germany.
11) "International Symposia on (e,2e) Double Photoionization and Related Topics & Polarization and Correlation in Electronic and Atomic Collisions", 30 July-1 August 2015, Universidad del Pais Vasco, San Sebastian, Spain.
12) "Advanced Workshop on High-Performance & High-Throughput Materials Simulations using QUANTUM ESPRESSO", 16-27 January 2017, Miramare, Trieste, Italy.
13) "New Computational Methods for Attosecond Molecular Processes", 21-25 May 2018, ZCAM, Zaragoza, Spain.
14) "Iterative Solvers for Linear Systems", 8-10 September 2021, Leibniz Supercomputer Center, Munich, Germany (online course).
15) "Ab initio many-body perturbation theory: from equilibrium to time-resolved spectroscopies and nonlinear optics", 22-26 May 2023, Rome, Italy.
16) "TREX Quantum Monte Carlo school" SISSA 3-7 July 2023, SISSA, Trieste, Italy.
17) "Advanced Quantum ESPRESSO school: Hubbard and Koopmans functionals from linear response", 28 August-1 September 2023, Pavia, Italy.

C. LANGUAGES

Italian (mother tongue), English (advanced level).

D. COMPUTATIONAL SKILLS

1) Operating systems: good knowledge of UNIX/LINUX, WINDOWS, and Mac-OS X.
2) Programming languages: good knowledge of FORTRAN77-FORTAN90/95, C++, parallel processing MPI e OpenMP.
3) Scientific software: ADF package, Gaussian09, MOLPRO, DALTON, GAMESS-US, ACESII, CFOUR, PWscf. Co-author of the MidasCpp software (prof. O. Christiansen, Aarhus University, DK), and software

for the calculation of photoionization and electron-molecule scattering processes developed in collaboration with prof. Piero Decleva, prof. Mauro Stener (Università degli Studi di Trieste) and prof. Robert R. Lucchese (Texas A&M University, USA).

PROFESSIONAL

A. APPOINTMENTS AT UNIVERSITIES/RESEARCH CENTERS

From 24/12/2017: Associate professor of Physical Chemistry, Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli studi di Trieste, Italy.
24/12/2014 – 23/12/2017: Assistant professor of Physical Chemistry, Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli studi di Trieste, Italy.
04/09/2008 – 23/12/2014: Assistant professor of Chemistry, Department of Chemistry, Middle East Technical University (METU), Ankara, Turkey.
01/09/2006 – 31/08/2008: Postdoctoral Research Associate, Department of Chemistry, University of Aarhus, Denmark.
02/05/2005 – 31/08/2006: Postdoctoral Research Associate, CNR-INFM Democritos, Italy.
01/02/2003 – 31/01/2005: Postdoctoral Research Associate, Department of Chemistry, Texas A&M University, USA.
01/01/2000 – 31/12/2002: PhD student, Dipartimento di Scienze Chimiche, Università degli studi di Trieste, Italy**.**

B. FELLOWSHIPS AND AWARDS

1) January 2022: Italian national habilitation to Full professor of Physical Chemistry.
2) January 2014: Italian national habilitation to Associate professor of Physical Chemistry.
3) October 2013: Associate professorship awarded by YOK (Higher Education Council, Turkey).
4) Shortlisted for a position of Assistant professor at the University of East Anglia (UK, 2011), and Wolverhampton (UK 2013).
5) Assistant professorship, Department of Chemistry, University of Aarhus, DK, 2008.
6) Postdoctoral Research Fellowship, Department of Chemistry, University of Aarhus, DK, 2006-2008.
7) Postdoctoral Fellowship of Ministerio de Ciencia y Innovación della Spagna, within the programme "Modalidad C: Estancias de jóvenes doctores extranjeros en universidades públicas y centros de investigación españoles", 2007-2008.
8) CNR-INFM postdoctoral research fellowship, 2005-2006.
9) Robert A. Welch Postdoctoral Fellowship, Houston, TX, USA, 2003-2005.
10) PhD fellowship, Università degli Studi di Trieste, 2000-2002.
11) Research fellowship, Università degli Studi di Udine, 2000.

C. REFEREEING ACTIVITY

Referee for the following journals: Physical Chemistry Chemical Physics (RSC), New Journal of Chemistry (RSC), Journal of Physical Chemistry (ACS), Journal of Chemical Theory and Computation (ACS), ACS Omega (ACS), Superlattices and Microstructures (Elsevier), Chemical Physics (Elsevier), Chemical Physics Letters (Elsevier), International Nanoletters (Springer), Journal of Physics B (IoP), Physica Scripta (IoP), Scientific Reports (Nature), Sensors (MDPI), Atmosphere (MDPI), Molecules (MDPI), Atoms (MDPI), Theoretical Chemistry Accounts (Wiley), Journal of Synchrotron Radiation (iUCr), Parallel Computing (Elsevier).

D. ORGANIZATION OF WORKSHOPS/CONFERENCES

1) Member of the scientific committee, "43th International Chemistry Olympiads", Ankara, 9-18 July 2011.
2) Member of the local organizing committee, "Turkish-Italian Workshop on the Frontiers in Nanomaterial Research and Application", Istanbul, 8-10 December 2010.
3) Member of the local organizing committee, "V Congresso della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana", Università degli studi di Trieste, Trieste, Italy, 19-21 September 2018.

E. FOUNDED NATIONAL AND INTERNATIONAL PROJECTS

1) Bilateral project TUBITAK (Turkish Council of Scientific and Technological Research)/CNR (Italia) Grant No. 209T083: "*Calculation of molecular multiphoton ionization cross sections*", principal investigator, (PI), 2010-2012.
2) Individual grant from METU (BAP-01-03-2009-101) "*Development of new algorithms for Molecular quantum dynamics, electron-molecule scattering and molecular photoionization*", 2009-2011.
3) TUBITAK Grant No. 108T706: "*Density functional theory investigation of NO_x storage/reduction catalysts*", 2009-2012 (Co-PI).
4) TUBITAK Grant No. 112T542: "*Density Functional Theory design of highly active catalysts for clean H_2 production for fuel-cell applications*", 2012-2014, PI.
5) TUBITAK Grant No. 113F099: "*Density Functional Theory investigation of the reaction mechanisms for selective oxidation of alcohols on gold catalysts*", 2013-2016, Co-PI.
6) Bilateral project TUBITAK/CNR Grant No. 113F377: "*Theoretical description of many-electron processes in photoionization*", 2014-2016 (local coordinator).
7) TUBITAK Grant No. 115F493: "*A joint theoretical and experimental study on nanotribological properties of the interface between Au and two-dimensional materials*", 2016-2018, external Co-PI with no funding.
8) Finanziamento per la Ricerca di Ateneo FRA 2015: "*Small molecules: keys for sustainable development*", 2016-2017, Co-PI.
9) NATO SPS (Science for Peace and Security Programme) G5195 Multi-Year Research Project "*Advanced Microwave Sources*", 2017-2020, Co-director.
10) Finanziamento per la Ricerca di Ateneo FRA 2018: "*Poliesteri funzionalizzati per applicazioni farmaceutiche e cosmetiche avanzate*", 2019-2020, Co-PI.
11) TUBITAK Grant No. 118F355: "*Theoretical modeling of single-atom catalysts on metal oxide surfaces*", 2019-2022, external Co-PI with no funding.
12) Funding for a departmental HPC cluster (35000 EUR from Stiftung Beneficentia fundation).
13) Funding for a post-doctoral fellowship POR FSE 2014/2020 (1yr, 20280.97 EUR).
14) Local coordinator for the "Piano Lauree Scientifiche (PLS)", specialty: Chemistry. Funded projects: PLS-2017-2018 (11 kEUR), PLS-2020 (11 kEUR), PLS-2021 (11 kEUR), PLS-2023- (16kEUR).

F. SUPERVISION OF STUDENTS/POSTDOCS

1) "EFFECT OF SUPPORT MATERIAL IN NOx STORAGE/REDUCTION CATALYSTS", Ruslan Hummatov, MSc in Physics 2010, METU, coadvisor.
2) "DENSITY FUNCTIONAL THEORY INVESTIGATION OF NOBLE METAL REDUCTION AGENTS ON GAMMA ALUMINIUM OXIDE IN NOx STORAGE/REDUCTION CATALYSTS", Zuleyha Artuç, MSc in Micro and Nano Technology 2011, METU, principal advisor.
3) "THE EFFECTS OF PROMOTERS ON THE SULFUR RESISTANCE OF NOx STORAGE/REDUCTION CATALYSTS: A DENSITY FUNCTIONAL THEORY INVESTIGATION", Rukan Koşak, MSc in Chemistry 2011, METU, principal advisor.
4) "AB INITIO MODELLING OF MATERIALS PROPERTIES FOR CATALYTIC AND DEVICE APPLICATIONS", Mehmet Gokhan Sensoy, PhD in Physics 2017, METU, coadvisor.
5) "PHYSICAL PROPERTIES OF ANATASE-TiO2 ALTERED BY LANTHANIDE ATOMS", Kivilcim Basak Vural, PhD in Physics 2015, METU, coadvisor.
6) Dr. Selma Bas (postdoc, 2012-2015).
7) "OPTICAL PROPERTIES OF NOBLE METAL NANOCLUSTERS STUDIED BY THE TIME DEPENDENT DENSITY FUNCTIONAL THEORY", Martina De Vetta, a.a. 2014-2015, MSc in Chemistry, Università degli Studi di Trieste, coadvisor.
8) "SPETTRI NEXAFS DI OLIGOMERI DELL'ACIDO FENILBORONICO IN FASE GASSOSA E SUPPORTATI SU Au(111). STUDIO COMPUTAZIONALE CON IL METODO DEL FUNZIONALE DENSITA' ", Elisa Bernes, a.a. 2014-2015, BSc in Chemistry, Università degli Studi di Trieste, coadvisor.
9) "APPLICAZIONE DEL METODO DFT AL CALCOLO DI SPETTRI NEXAFS DI DERIVATI TETRAZOLICI IN FASE GASSOSA", Silvia Mauri a.a. 2015-2016, BSc in Chemistry, Università degli Studi di Trieste, coadvisor.
10) "SIMULAZIONE DI SPETTRI C1s NEXAFS E XPS DI IDROCARBURI POLICICLICI AROMATICI IN FASE GASSOSA", Emanuele Rossi, a.a. 2016-2017, BSc in Chemistry, Università degli Studi di Trieste, coadvisor.
11) "SIMULAZIONE DI SPETTRI C1s NEXAFS E XPS DI IDROCARBURI POLIINSATURI IN FASE GASSOSA", Nicolas Fonda, a.a. 2016-2017, BSc in Chemistry, Università degli Studi di Trieste, coadvisor.

12) "SIMULAZIONE DI SPETTRI C1s NEXAFS E XPS DI AZULENE E 6,6 DIMETIL FULVENE IN FASE GASSOSA", Mark Colbassi, a.a. 2016-2017, BSc in Chemistry, Università degli Studi di Trieste, coadvisor.
13) "SPETTRI C1s NEXAFS E XPS DEL TIOFENE E DI SUOI BENZO—DERIVATI: STUDIO COMPUTAZIONALE CON IL METODO DEL FUNZIONALE DENISTA' ", Andrea Greselin, a.a. 2016-2017, BSc in Chemistry, Università degli Studi di Trieste, coadvisor.
14) "SPETTROSCOPIE DI CORE PER L'ANALISI DELLA STRUTTURA ELETTRONICA DI NETWORK BORONICI SU SUPERFICI METALLICHE", Nicola Danielis, a.a. 2017-2018, BSc in Chemistry, Università degli Studi di Trieste, coadvisor.
15) "STUDI NEXAFS E XPS DI MOLECOLE MODELLO PER IL GRAFENE DROGATO CON AZOTO", Lia Visintin, a.a. 2017-2018, BSc in Chemistry, Università degli Studi di Trieste, coadvisor.
16) "EFFETTI CONFORMAZIONALI SU SPETTRI ELETTRONICI DI CORE DI DERIVATI DELL' OSSIDO DELLA TRIFENILFOSFINA", Miriam Marchi, a.a. 2017-2018, BSc in Chemistry, Università degli Studi di Trieste, coadvisor.
17) "SPETTRI NEXAFS DELLA TITANIL-FTALOCIANINA: STUDIO COMPUTAZIONALE CON IL METODO DEL FUNZIONALE DENSITA'", Chiara Morassut, a.a. 2018-2019, BSc in Chemistry, Università degli Studi di Trieste, advisor.
18) "ACIDO NAFTALENBORONICO (NBA) COME PRECURSORE DI FRAMEWORKS 2D SU SUPERFICI DI Au(111): STUDIO COMPUTAZIONALE DEGLI SPETTRI DI CORE", Elena Zerbato, a.a. 2018-2019, BSc in Chemistry, Università degli Studi di Trieste, coadvisor.
19) "CORE EXCITATION SPECTRA OF 2D BOROXINE-CONTAINING FRAMEWORKS DEPOSITED ON THE Au(111) SURFACE: A COMPUTATIONAL INVESTIGATION", Dr. Silvia Mauri, a.a. 2017-2018, MSc in Chemistry, Università degli Studi di Trieste, advisor.
20) "COMPUTATIONAL STUDY OF THE CIRCULAR DICHROISM IN PLASMONIC CHIRAL GOLD NANOTUBES", Andrea Russi, a.a. 2019-2020, MSc in Chemistry, Università degli Studi di Trieste, coadvisor.
21) "FRAMEWORKS 2D OTTENUTI DALLA CONDENSAZIONE DELL'ACIDO NAFTALENBORONICO: STUDIO DEGLI EFFETTI STRUTTURALI SUGLI SPETTRI NEXAFS DI SISTEMI MODELLO", Gabriele Fabbro, a.a. 2019-2020, BSc in Chemistry, Università degli Studi di Trieste, advisor.
22) "SIMULATION OF CORE-ELECTRON SPECTROSCOPIES OF GAS-PHASE MOLECULES AND ADSORBATES BY DFT AND TDDFT METHODS", Dr. Elisa Bernes, a.a. 2017-2020, PhD in Chemistry, Università degli Studi di Trieste, advisor.
23) "APPLICAZIONI DI METODI DFT E TDDFT AL CALCOLO DELLE ECCITAZIONI DI VALENZA DI DERIVATI DEL BODIPY", Matteo Quarin, a.a. 2021-2022 BSc in Chemistry, Università degli Studi di Trieste, advisor.
24) "PROPRIETA' ELETTRONICHE DELL'INTERFACCIA TRA TRIPIRENBOROSSINA E Au(111)", Simone Micheloni, a.a. 2022-2023 MSc in Chemistry, Università degli Studi di Trieste, co-advisor.
25) "PLASMONIC COUPLING EFFECT OF SILVER/GOLD/COPPER CLUSTERS SUPPORTED OVER TiO2: A THEORETICAL STUDY", Sènoumè Parfaite Senou, MSc in Chemistry, Sorbonne Université, Parigi, 2023.

DEPARTMENTAL/UNIVERSITY SERVICE

1) Member of the committee for the students' admission to the PhD program in Chemistry (July 2016)
2) Member of the education committee for the undergraduate curriculum program in Chemistry (2017-ongoing)
3) Member of the board of doctoral studies (2018-2021)
4) Local coordinator (Chemistry) of the "Progetto Lauree Scientifiche" (2018-ongoing)
5) Member of the "commissione per gli esami di stato di abilitazione alla professione di Chimico" (state exam for the habilitation to chemistry professionals) (2018)
6) Department representative for the interdepartmental STeDIC HPC center of UniTS (2018-2021).
7) Coordinator of the STeDIC interdepartmental HPC center of UniTS (2022-ongoing).
8) Member of the departmental commission AQ "Assicurazione della Qualità" (2018-2021)
9) Member of the evaluation committee for a position of associate professor in physical chemistry (UniTS, 2019, 2021)
10) Member of the evaluation committee for a position of assistant professor (RTD-A) in physical chemistry (UniVE, 2018, UniTS, 2022)
11) External evaluator of the PhD thesis of Mr Shawkat Islam (2018, Swinburne University of Technology, Victoria, AUS)
12) Member of the evaluation committee for the assignment of tutoring activities for MSc and PhD students

(2017-ongoing) and fellowships (prizes, and postdocs).
13) Referee for VQR 2015-2019 of National Agency for the Evaluation of Universities and Research Institutes (ANVUR)

TEACHING ACTIVITY

A. UNDERGRADUATE/GRADUATE COURSES

1) "CHEM107 – GENERAL CHEMISTRY FOR ENGINEERS" (ECTS credits: 6.0): a.a. 2008-2009 (I semester, II semester), a.a. 2014-2015 (I semester), METU.
2) "CHEM252 – PHYSICAL CHEMISTRY I" (ECTS credits: 7.0): a.a 2013-2014 (II semester), METU.
3) "CHEM254 – PHYSICAL CHEMISTRY LABORATORY I" (ECTS credits: 6.0), a.a 2013-2014 (II semester), METU.
4) "CHEM257 – MATHEMATICS FOR CHEMISTS" (ECTS credits: 7.5), a.a. 2009-2010 (I semester, II semestre, sessione straordinaria estiva), a.a. 2010-2011 (I semester) a.a. 2011-2012 (I semester), a.a. 2012-2013 (I semester) a.a. 2013-2014 (I semester), METU.
5) "CHEM489 – COMPUTATIONAL CHEMISTRY" (ECTS credits: 7.5), a.a. 2008-2009 (II semester), a.a. 2009-2010 (II semester), METU (new class designed for undergrads in Chemistry and Physics).
6) "CHEM597 – ADVANCED TOPICS IN PHYSICAL CHEMISTRY" (ECTS credits: 8.0), a.a. 2009-2010 (I semester), a.a. 2010-2011 (II semester), a.a. 2011-2012 (II semester), a.a. 2012-2013 (II semester), a.a. 2013-2014 (II semester), METU.
7) "CHEM111 – GENERAL CHEMISTRY I" (ECTS credits: 6.0), a.a. 2010-2011 (I semester), a.a. 2011-2012 (I semester), a.a. 2012-2013 (I semester), a.a. 2013-2014 (I semester), a.a. 2014-2015 (I semester), METU.
8) "CHEM112 – GENERAL CHEMISTRY II" (ECTS credits: 6.0), a.a. 2011-2012 (II semester), 2011-2013 (II semester), METU.
9) "CHEM429 – SIMULATION TECHNIQUES IN THEORETICAL CHEMISTRY" (ECTS credits: 7.5), a.a. 2010-2011 (II semester), METU (new class designed for undergrads in Chemistry and Physics).
10) 108SM – APPLICAZIONI CHIMICHE DELLA SIMMETRIA MOLECOLARE (4 CFU), a.a. 2015-2016, a.a. 2016-2017, Università degli studi di Trieste.
11) 691SM – CHIMICA FISICA IV e CHIMICA FISICA DEI SOLIDI (3 CFU), a.a. 2016-2017, Università degli studi di Trieste.
12) 080SM – CHIMICA FISICA I CON LABORATORIO (12 CFU), from a.a. 2017-2018, Università degli Studi di Trieste.

B. OTHER TEACHING ACTIVITIES

1) Lecturer at the "Summer School on Modelling Nanostructures using Density Functional Theory", Izmir, Turkey, 10-21 August 2009
2) Lecturer at the "International Winter School on Physics and Chemistry of Solids: Theory and Experiment", Ankara, Turkey, 6-12 November 2011
3) Lecturer, "Calculation of molecular unbound states", Mid-Term Check COSINE ITN network, May 22-23 2019 Trieste, Italy

PUBLICATION 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) L. Randaccio, S. Geremia, M. Stener, D. Toffoli and E. 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) D. Toffoli and R. 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) D. Toffoli, M. J. Simpson and R. 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. Erratum: The Journal of Chemical Physics **131**(16), Art. No 169901 (1 page)
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) D. Toffoli, R. 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 property 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) M. B. Hansen, O. Christiansen, D. Toffoli, and J. 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) M. B. Hansen, J. Kongsted, D. Toffoli, and O. 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, 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**(22), 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 (10 pages), 2008.
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INVITED TALKS, PROCEEDINGS, ORAL AND POSTER PREASENTATIONS AT NATIONAL AND INTERNATIONAL CONGRESSES/WORKSHOPS (PARTIAL)

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