Daniele Toffoli

List of Publications by Year
in descending order

103	3,502	304743 22	138484 58
papers	citations	h-index	g-index

105	105	105	3679
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Continuum Electronic States: The Tiresia Code. Molecules, 2022, 27, 2026.	3.8	9
2	Plasmonic Circular Dichroism in Chiral Gold Nanowire Dimers. Molecules, 2022, 27, 93.	3.8	5
3	Computational NEXAFS Characterization of Molecular Model Systems for 2D Boroxine Frameworks. Nanomaterials, 2022, 12, 1610.	4.1	1
4	Tribology at the atomic scale with density functional theory. Electronic Structure, 2022, 4, 023002.	2.8	3
5	Temperature-dependent thermoelastic properties of GaSb and InSb semiconductors: Identification through ab initio DFT simulations. Physica B: Condensed Matter, 2022, 643, 414135.	2.7	3
6	Revealing the electronic properties of the Bâ€“B bond: the bis-catecholato diboron molecule. Physical Chemistry Chemical Physics, 2021, 23, 23517-23525.	2.8	2
7	Theoretical Investigation of Photoinduced Processes in Subnanometer Oxide-Supported Metal Catalysts. Journal of Physical Chemistry C, 2021, 125, 2022-2032.	3.1	4
8	Polymer interfaces with carbon nanostructures: First principles density functional theory and molecular dynamics study of polyetheretherketone adsorption on graphene and nanotubes. Computational Materials Science, 2021, 191, 110320.	3.0	5
9	Carbon and Nitrogen K-Edge NEXAFS Spectra of Indole, 2,3-Dihydro-7-azaindole, and 3-Formylindole. Journal of Physical Chemistry A, 2021, 125, 4160-4172.	2.5	4
10	Formaldehyde Selectivity in Methanol Partial Oxidation on Silver: Effect of Reactive Oxygen Species, Surface Reconstruction, and Stability of Intermediates. ACS Catalysis, 2021, 11, 6200-6209.	11.2	14
11	Circularly Polarized Plasmons in Chiral Gold Nanowires via Quantum-Mechanical Design. Journal of Physical Chemistry Letters, 2021, 12, 5829-5835.	4.6	4
12	Predictive optical photoabsorption of Ag24Au(DMBT)18â^' via efficient TDDFT simulations. Journal of Chemical Physics, 2021, 155, 084103.	3.0	12
13	Time-Resolved Excited-State Analysis of Molecular Electron Dynamics by TDDFT and Betheâ€“Salpeter Equation Formalisms. Journal of Chemical Theory and Computation, 2021, 17, 6314-6329.	5.3	8
14	Î²-Fluorinated Paraconic Acid Derivatives: Synthesis and Fluorine Stereoelectronic Effects. Journal of Fluorine Chemistry, 2021, 249, 109860.	1.7	0
15	On-Surface Synthesis of Boroxine-Based Molecules. Chemistry, 2021, 3, 1401-1410.	2.2	2
16	First-principles investigation of CO and CO2 adsorption on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si61.svg"><mml:mrow><mml:mi>Î³</mml:mi></mml:mrow></mml:math>-Al2O3 supported monoatomic and diatomic Pt clusters. Applied Surface Science, 2020, 499, 143968.	6.1	10
17	S 2p and P 2p Core Level Spectroscopy of PPT Ambipolar Material and Its Building Block Moieties. Journal of Physical Chemistry C, 2020, 124, 14510-14520.	3.1	3
18	Methylamine terminated molecules on Ni(1 1 1): A path to low temperature synthesis of nitrogen-doped graphene. FlatChem, 2020, 24, 100205.	5.6	4

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19	Photoionization Dynamics of the Tetraoxo Complexes OsO₄ and RuO₄. Inorganic Chemistry, 2020, 59, 7274-7282.	4.0	2
20	PPT Isolated Molecule and Its Building Block Moieties Studied by C 1s and O 1s Gas Phase X-ray Photoelectron and Photoabsorption Spectroscopies. Journal of Physical Chemistry C, 2020, 124, 9774-9786.	3.1	4
21	An efficient hybrid scheme for time dependent density functional theory. Journal of Chemical Physics, 2020, 152, 184104.	3.0	10
22	Angular dependent time delay near correlation induced Cooper minima. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 115201.	1.5	9
23	Experimental and Theoretical Photoemission Study of Indole and Its Derivatives in the Gas Phase. Journal of Physical Chemistry A, 2020, 124, 4115-4127.	2.5	19
24	Nanotribological Properties of the h-BN/Au(111) Interface: A DFT Study. Journal of Physical Chemistry C, 2019, 123, 28411-28418.	3.1	10
25	Combined effect of point defects and layer number on the adsorption of benzene and toluene on graphene. Applied Surface Science, 2019, 480, 1063-1069.	6.1	12
26	Correlation effects in B1s core-excited states of boronic-acid derivatives: An experimental and computational study. Journal of Chemical Physics, 2019, 151, 134306.	3.0	4
27	Pd doping, conformational, and charge effects on the dichroic response of a monolayer protected Au₃₈(SR)₂₄ nanocluster. Physical Chemistry Chemical Physics, 2019, 21, 3585-3596.	2.8	6
28	Chirality in bare and ligand-protected metal nanoclusters. Advances in Physics: X, 2018, 3, 1509727.	4.1	21
29	Electronic Structure Characterization of a Thiophene Benzo-Annulated Series of Common Building Blocks for Donor and Acceptor Compounds Studied by Gas Phase Photoelectron and Photoabsorption Synchrotron Spectroscopies. Journal of Physical Chemistry A, 2018, 122, 8745-8761.	2.5	4
30	Instability of a Noncrystalline NaO₂ Film in Naâ€“O₂ Batteries: The Controversial Effect of the RuO₂ Catalyst. Journal of Physical Chemistry C, 2018, 122, 19678-19686.	3.1	7
31	Timeâ€dependent densityâ€functional study of the photoabsorption spectrum of Au₂₅(SC₂H₄C₆H₅)₁₈ anion: Validation of the computational protocol. International Journal of Quantum Chemistry, 2018, 118, e25769.	2.0	9
32	Individual Component Map of Rotatory Strength and Rotatory Strength Density Plots As Analysis Tools of Circular Dichroism Spectra of Complex Systems. Journal of Chemical Theory and Computation, 2018, 14, 3703-3714.	5.3	13
33	Electronic properties of the boroxineâ€“gold interface: evidence of ultra-fast charge delocalization. Chemical Science, 2017, 8, 3789-3798.	7.4	18
34	Structural and electronic properties of bulk and low-index surfaces of zincblende PtC. Journal of Physics Condensed Matter, 2017, 29, 125002.	1.8	2
35	Effect of Platinum, Gold, and Potassium Additives on the Surface Chemistry of CdI₂-Antitype Mo₂C. ACS Omega, 2017, 2, 7976-7984.	3.5	2
36	S2p core level spectroscopy of short chain oligothiophenes. Journal of Chemical Physics, 2017, 147, 244301.	3.0	10

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37	Interference effects in photoelectron asymmetry parameter (Î²) trends of C 2sâ^'1states of ethyne, ethene and ethane. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 235102.	1.5	2
38	Extension of the Time-Dependent Density Functional Complex Polarizability Algorithm to Circular Dichroism: Implementation and Applications to Ag₈ and Au₃₈(SC₂H₄C₆H₅)₂₄. Journal of Physical Chemistry C, 2016, 120, 24335-24345.	3.1	14
39	A Multichannel Least-Squares B-Spline Approach to Molecular Photoionization: Theory, Implementation, and Applications within the Configurationâ€“Interaction Singles Approximation. Journal of Chemical Theory and Computation, 2016, 12, 4996-5008.	5.3	34
40	Comparative Analysis of Reactant and Product Adsorption Energies in the Selective Oxidative Coupling of Alcohols to Esters on Au(111). Topics in Catalysis, 2016, 59, 1383-1393.	2.8	3
41	Photoelectron diffraction in methane probed via vibrationally resolved inner-valence photoionization cross-section ratios. Physical Chemistry Chemical Physics, 2016, 18, 3214-3222.	2.8	4
42	Multiscale Self-Assembly of Silicon Quantum Dots into an Anisotropic Three-Dimensional Random Network. Nano Letters, 2016, 16, 1942-1948.	9.1	9
43	Active role of the support in NO x storage and reductioncatalytic systems. Applied Surface Science, 2015, 355, 1295-1305.	6.1	2
44	Dynamical effects in the vibrationally resolved C 2s⁻¹ photoionization cross section ratios of Methane. Journal of Physics: Conference Series, 2015, 635, 112048.	0.4	0
45	Covalent and noncovalent functionalization of pristine and defective graphene by cyclohexane and dehydrogenated derivatives. Applied Surface Science, 2015, 351, 344-352.	6.1	14
46	Understanding the Effects of Ion-Exchange in Titanosilicate ETS-10: A Joint Theoretical and Experimental Study. Journal of Physical Chemistry C, 2014, 118, 27281-27291.	3.1	8
47	Effect of ion-exchange on Structural, Electronic, and Vibrational Properties of the -O-Ti-O-Ti-O- Quantum Wires in ETS-10. Materials Research Society Symposia Proceedings, 2014, 1704, 1.	0.1	0
48	Electrochromic properties of multicolored novel polymer synthesized via combination of benzotriazole and N-functionalized 2,5-di(2-thienyl)-1H-pyrrole units. Electrochimica Acta, 2014, 138, 454-463.	5.2	20
49	First principles investigation of NO2 and SO2 adsorption on Î³-Al2O3 supported mono- and diatomic metal clusters. RSC Advances, 2014, 4, 48492-48506.	3.6	3
50	Insights into surfaceâ€“adsorbate interactions in corrosion inhibition processes at the molecular level. Corrosion Science, 2014, 80, 482-486.	6.6	47
51	Bis(triisopropylsilylethynyl)pentacene/Au(111) Interface: Coupling, Molecular Orientation, and Thermal Stability. Journal of Physical Chemistry C, 2014, 118, 22522-22532.	3.1	10
52	Ab initio potential energy and dipole moment surfaces of the Fâ^'(H2O) complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 119, 59-62.	3.9	20
53	Density functional theory investigation of two-dimensional dipolar fermions in a harmonic trap. Journal of Physics: Conference Series, 2014, 568, 012020.	0.4	7
54	Further investigation of intramolecular H-bonding in benzimidazole and EDOT containing monomer. Journal of Electroanalytical Chemistry, 2013, 693, 23-27.	3.8	6

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55	Multiphoton core ionization dynamics of polyatomic molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2013, 46, 145101.	1.5	5
56	Appearance of Plasmons in Fullerenes. Journal of Physics: Conference Series, 2012, 388, 022087.	0.4	2
57	Density functional theory for molecular multiphoton ionization in the perturbative regime. Journal of Chemical Physics, 2012, 137, 134103.	3.0	11
58	First-Principles Investigation of NO_x and SO_x Adsorption on Anatase-Supported BaO and Pt Overlayers. Journal of Physical Chemistry C, 2012, 116, 6191-6199.	3.1	20
59	The valence electronic structure and conformational flexibility of epichlorohydrin. Physical Chemistry Chemical Physics, 2011, 13, 12517.	2.8	5
60	Computational characterization of the HOMO-2 photoemission intensity oscillations in C60. Chemical Physics Letters, 2011, 516, 154-157.	2.6	9
61	Vibrational spectroscopy of hydrogen-bonded systems: Six-dimensional simulation of the IR spectrum of Fâ^'(H2O) complex. Chemical Physics Letters, 2011, 510, 36-41.	2.6	10
62	Shape and Feshbach resonances in inner-shell photodetachment of negative ions. Journal of Electron Spectroscopy and Related Phenomena, 2011, 183, 64-69.	1.7	4
63	Accurate multimode vibrational calculations using a B-spline basis: theory, tests and application to dioxirane and diazirinone. Molecular Physics, 2011, 109, 673-685.	1.7	33
64	Partial photoionization cross sections of C60 and C70: A gas versus adsorbed phase comparison. Surface Science, 2010, 604, 1940-1944.	1.9	13
65	Vibrational absorption spectra calculated from vibrational configuration interaction response theory using the Lanczos method. Journal of Chemical Physics, 2010, 132, 164105.	3.0	26
66	Strong oscillations in the nondipole corrections to the photoelectron angular distributions fromC60. Physical Review A, 2010, 81, .	2.5	14
67	Metallization of the C60/Rh(100) interface revealed by valence photoelectron spectroscopy and density functional theory calculations. Journal of Chemical Physics, 2010, 132, 234710.	3.0	5
68	Using Electronic Energy Derivative Information in Automated Potential Energy Surface Construction for Vibrational Calculations. Journal of Chemical Theory and Computation, 2010, 6, 3162-3175.	5.3	39
69	New Formulation and Implementation of Vibrational Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2010, 6, 235-248.	5.3	69
70	A hierarchy of potential energy surfaces constructed from energies and energy derivatives calculated on grids. Journal of Chemical Physics, 2009, 130, 134104.	3.0	30
71	An adaptive density-guided approach for the generation of potential energy surfaces of polyatomic molecules. Theoretical Chemistry Accounts, 2009, 123, 413-429.	1.4	73
72	Potential Energy Surfaces for Vibrational Structure Calculations from a Multiresolution Adaptive Density-Guided Approach: Implementation and Test Calculations. Journal of Physical Chemistry A, 2009, 113, 8712-8723.	2.5	34

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73	Vibrational Contributions to Indirect Spinâ^'Spin Coupling Constants Calculated via Variational Anharmonic Approaches. Journal of Physical Chemistry A, 2008, 112, 8436-8445.	2.5	17
74	A virtual vibrational self-consistent-field method for efficient calculation of molecular vibrational partition functions and thermal effects on molecular properties. Journal of Chemical Physics, 2008, 128, 174106.	3.0	21
75	A multicentric approach to the calculation of nondipolar effects in molecular photoemission. Journal of Chemical Physics, 2008, 128, 234101.	3.0	8
76	Nondipolar effects in the photoionization dynamics of carbon tetrafluoride. Physical Review A, 2008, 78, .	2.5	2
77	The dipole and non-dipole parameters of the N K shell of the N₂molecule up to 80 eV above threshold. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 221002.	1.5	4
78	Spinâ€“orbit-activated interchannel coupling in the 3d photoionization of barium atoms. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 4005-4012.	1.5	3
79	Molecular frame and recoil frame photoelectron angular distributions from dissociative photoionization of NO2. Journal of Chemical Physics, 2007, 126, 054307.	3.0	35
80	Automatic generation of potential energy and property surfaces of polyatomic molecules in normal coordinates. Journal of Chemical Physics, 2007, 127, 204106.	3.0	54
81	Shape resonances in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>K</mml:mi></mml:math>-shell photodetachment of small size-selected clusters: Experiment and theory. Physical Review A, 2007, 76, .	2.5	6
82	Defect-Controlled Transport Properties of Metallic Atoms along Carbon Nanotube Surfaces. Physical Review Letters, 2007, 99, 046803.	7.8	31
83	Density functional theory for the photoionization dynamics of uracil. Journal of Chemical Physics, 2007, 127, 234317.	3.0	15
84	Recent advances in molecular photoionization by density functional theory based approaches. Theoretical Chemistry Accounts, 2007, 117, 943-956.	1.4	34
85	Time dependent density functional investigation of the near-edge absorption spectra of V2O5. Physical Chemistry Chemical Physics, 2006, 8, 4300.	2.8	23
86	Time dependent density functional study of the photoionization dynamics of SF6. Journal of Chemical Physics, 2006, 124, 114306.	3.0	28
87	Photoelectron angular distributions beyond the dipole approximation: a computational study on the N2molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, 2681-2691.	1.5	25
88	Photoabsorption and photoionization dynamics study of silicon tetrafluoride in the framework of time-dependent density-functional theory. Physical Review A, 2006, 73, .	2.5	6
89	Photoionization cross section and angular distribution calculations of carbon tetrafluoride. Journal of Chemical Physics, 2006, 124, 214313.	3.0	10
90	Photoelectron trapping in N2O 7Ïƒâ†'kÏƒ resonant ionization. Journal of Chemical Physics, 2005, 123, 014307.	3.0	12

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91	Near threshold photoionization of the ground and first excited states of C2. Journal of Chemical Physics, 2004, 120, 6010-6018.	3.0	12
92	Cross-section and asymmetry-parameter calculations for the outer- and inner-valence photoionization of ethane. Physical Review A, 2004, 69, .	2.5	4
93	Symmetry- and multiplet-resolved N1sphotoionization cross sections of theNO2molecule. Physical Review A, 2004, 70, .	2.5	11
94	A tunable carbon nanotube electromechanical oscillator. Nature, 2004, 431, 284-287.	27.8	1,194
95	Electronâ^'Phonon Scattering in Metallic Single-Walled Carbon Nanotubes. Nano Letters, 2004, 4, 517-520.	9.1	676
96	Least squares B-spline solutions of the radial Dirac equation in the continuum. Computer Physics Communications, 2003, 152, 151-164.	7.5	0
97	3d photoionization along the xenon isoelectronic sequence. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 3097-3118.	1.5	6
98	Photoionization of mercury: A relativistic time-dependent density-functional-theory approach. Physical Review A, 2002, 66, .	2.5	17
99	Valence and core photoemission in M@C60(M = Be, Mg, Ca). Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 1421-1438.	1.5	33
100	Electronic Properties of the Axial Coâ^'C and Coâ^'S Bonds in B12 Systems â^' A Density Functional Study. European Journal of Inorganic Chemistry, 2002, 2002, 93-103.	2.0	36
101	Convergence of the multicenter B-spline DFT approach for the continuum. Chemical Physics, 2002, 276, 25-43.	1.9	129
102	Time dependent density functional photoionization of CH4, NH3, H2O and HF. Chemical Physics, 2002, 282, 337-351.	1.9	48
103	Similarities and Differences between Cobalamins and Cobaloximes. Accurate Structural Determination of Methylcobalamin and of LiCl- and KCl-Containing Cyanocobalamins by Synchrotron Radiation. Inorganic Chemistry, 2000, 39, 3403-3413.	4.0	134