Francesco Tarantelli

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3010440/publications.pdf

Version: 2024-02-01

221	7,879	50276	71685
papers	citations	46 h-index	76 g-index

226	226	226	4742
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Giant Intermolecular Decay and Fragmentation of Clusters. Physical Review Letters, 1997, 79, 4778-4781.	7.8	634
2	The Chemical Bond between Au(I) and the Noble Gases. Comparative Study of NgAuF and NgAu⁺ (Ng = Ar, Kr, Xe) by Density Functional and Coupled Cluster Methods. Journal of the American Chemical Society, 2008, 130, 1048-1060.	13.7	260
3	Influence of the dye molecular structure on the TiO₂conduction band in dye-sensitized solar cells: disentangling charge transfer and electrostatic effects. Energy and Environmental Science, 2013, 6, 183-193.	30.8	247
4	Auger Electron Angular Distribution of Double Core-Hole States in the Molecular Reference Frame. Physical Review Letters, 2010, 105, 083004.	7.8	163
5	On double vacancies in the core. Journal of Chemical Physics, 1986, 85, 6513-6523.	3.0	160
6	How Ï€ back-donation quantitatively controls the CO stretching response in classical and non-classical metal carbonyl complexes. Chemical Science, 2016, 7, 1174-1184.	7.4	158
7	Double Core-Hole Production in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>: Beating the Auger Clock. Physical Review Letters, 2010, 105, 083005.	7.8	155
8	Ion Pairing in Cationic Olefinâ^'Gold(I) Complexes. Journal of the American Chemical Society, 2009, 131, 3170-3171.	13.7	134
9	Block Lanczos and manyâ€body theory: Application to the oneâ€particle Greenâ€™s function. Journal of Chemical Physics, 1996, 104, 7122-7138.	3.0	131
10	pKa of zinc-bound water and nucleophilicity of hydroxo-containing species. Ab initio calculations on models for zinc enzymes. Inorganic Chemistry, 1990, 29, 1460-1463.	4.0	114
11	Nuclear dynamics of decaying states: A timeâ€dependent formulation. Journal of Chemical Physics, 1993, 98, 9691-9706.	3.0	107
12	Revealing Charge-Transfer Effects in Gas-Phase Water Chemistry. Accounts of Chemical Research, 2012, 45, 1571-1580.	15.6	107
13	Solvent-, Silver-, and Acid-Free NHC-Au-X Catalyzed Hydration of Alkynes. The Pivotal Role of the Counterion. ACS Catalysis, 2016, 6, 7363-7376.	11.2	106
14	Theoretical investigation of many dicationic states and the Auger spectrum of benzene. Journal of Chemical Physics, 1987, 86, 2201-2206.	3.0	103
15	Counterion Effect in the Reaction Mechanism of NHC Gold(I)-Catalyzed Alkoxylation of Alkynes: Computational Insight into Experiment. ACS Catalysis, 2015, 5, 803-814.	11.2	98
16	A Phosphine Gold(I) Ï€-Alkyne Complex: Tuning the Metalâ^'Alkyne Bond Character and Counterion Position by the Choice of the Ancillary Ligand. Inorganic Chemistry, 2010, 49, 3080-3082.	4.0	92
17	On the Dewarâ€“Chattâ€“Duncanson Model for Catalytic Gold(I) Complexes. Chemistry - A European Journal, 2010, 16, 7231-7240.	3.3	91
18	Many dicationic states and twoâ€hole population analysis as a bridge to Auger spectra: Strong localization phenomena in BF3. Journal of Chemical Physics, 1991, 94, 523-532.	3.0	84

#	Article	IF	Citations
19	Charge-Transfer Energy in the Waterâ^'Hydrogen Molecular Aggregate Revealed by Molecular-Beam Scattering Experiments, Charge Displacement Analysis, and ab Initio Calculations. Journal of the American Chemical Society, 2010, 132, 13046-13058.	13.7	80
20	Ligand Effects on Bonding and Ion Pairing in Cationic Gold(I) Catalysts Bearing Unsaturated Hydrocarbons. European Journal of Inorganic Chemistry, 2013, 2013, 4121-4135.	2.0	73
21	The Chemical Bond in Gold(I) Complexes with N-Heterocyclic Carbenes. Organometallics, 2014, 33, 4200-4208.	2.3	73
22	Charge-displacement analysis via natural orbitals for chemical valence: Charge transfer effects in coordination chemistry. Journal of Chemical Physics, 2015, 142, 084112.	3.0	69
23	Dicationic states of hydrocarbons and a statistical approach to their Auger spectra. Journal of Chemical Physics, 1990, 92, 2984-2999.	3.0	68
24	When the Tolman Electronic Parameter Fails: A Comparative DFT and Charge Displacement Study of [(L)Ni(CO)₃]^{0/â€“} and [(L)Au(CO)]^{0/+}. Inorganic Chemistry, 2014, 53, 9907-9916.	4.0	67
25	Double vacancies in the core of benzene. Journal of Chemical Physics, 1987, 86, 2168-2175.	3.0	65
26	Unexpected Anion Effect in the Alkoxylation of Alkynes Catalyzed by Nâ€Heterocyclic Carbene (NHC) Cationic Gold Complexes. Chemistry - A European Journal, 2014, 20, 14594-14598.	3.3	63
27	Disentanglement of Donation and Backâ€Donation Effects on Experimental Observables: A Case Study of Goldâ€“Ethyne Complexes. Angewandte Chemie - International Edition, 2013, 52, 11599-11602.	13.8	61
28	Extensive Experimental and Computational Study of Counterion Effect in the Reaction Mechanism of NHC-Gold(I)-Catalyzed Alkoxylation of Alkynes. Organometallics, 2016, 35, 641-654.	2.3	61
29	Highly excited electronic states of molecular clusters and their decay. Journal of Chemical Physics, 1998, 108, 9737-9750.	3.0	60
30	On the doubly ionized states of ammonia. Chemical Physics Letters, 1985, 117, 577-582.	2.6	59
31	Foreign imaging in Auger spectroscopy: The Si 2pspectrum of silicon tetrafluoride. Physical Review Letters, 1993, 71, 649-652.	7.8	59
32	Recent advances and perspectives in four-component Diracâ€“Kohnâ€“Sham calculations. Physical Chemistry Chemical Physics, 2011, 13, 12368.	2.8	59
33	Band shape and vibrational structure in Auger spectra: Theory and application to carbon monoxide. Journal of Chemical Physics, 1991, 95, 6634-6644.	3.0	57
34	An ab Initio Benchmark and DFT Validation Study on Gold(I)-Catalyzed Hydroamination of Alkynes. Journal of Chemical Theory and Computation, 2014, 10, 1021-1034.	5.3	57
35	NHC-Gold-Alkyne Complexes: Influence of the Carbene Backbone on the Ion Pair Structure. Organometallics, 2013, 32, 4444-4447.	2.3	56
36	A Quantitative View of Charge Transfer in the Hydrogen Bond: The Water Dimer Case. ChemPhysChem, 2014, 15, 2682-2687.	2.1	55

#	Article	IF	Citations
37	Molecular-Beam Scattering Experiments and Theoretical Calculations Probing Charge Transfer in Weakly Bound Complexes of Water. Journal of Physical Chemistry A, 2009, 113, 15223-15232.	2.5	53
38	Selectively Measuring Ï€â€…Backâ€Donation in Gold(I) Complexes by NMR Spectroscopy. Chemistry - A European Journal, 2015, 21, 2467-2473.	3.3	53
39	Experimental Evidence of Chemical Components in the Bonding of Helium and Neon with Neutral Molecules. Chemistry - A European Journal, 2015, 21, 6234-6240.	3.3	53
40	Experimental and theoretical evidence of charge transfer in weakly bound complexes of water. Physical Chemistry Chemical Physics, 2009, 11, 9970.	2.8	52
41	Doubly ionized states of ethylene: Auger spectrum, potential energy surfaces and nuclear dynamics. Journal of Chemical Physics, 1989, 91, 1734-1753.	3.0	51
42	Evidence of a Borderline Region between E1cb and E2 Elimination Reaction Mechanisms:Â A Combined Experimental and Theoretical Study of Systems Activated by the Pyridine Ring. Journal of the American Chemical Society, 2005, 127, 15151-15160.	13.7	50
43	A Greenâ€™s function and configuration interaction investigation on the doubly ionized states of H2O. Journal of Chemical Physics, 1985, 83, 4683-4690.	3.0	49
44	Nuclear dynamics of several decaying overlapping electronic states: A timeâ€dependent formulation. Journal of Chemical Physics, 1993, 99, 5871-5884.	3.0	49
45	The calculation of molecular double ionization spectra by Greenâ€™s functions. Chemical Physics, 2006, 329, 11-21.	1.9	49
46	Ï€ Activation of Alkynes in Homogeneous and Heterogeneous Gold Catalysis. Journal of Physical Chemistry A, 2016, 120, 5239-5247.	2.5	49
47	Controlled Interplay between Decay and Fragmentation in Resonant Auger Processes. Physical Review Letters, 1998, 80, 1865-1868.	7.8	48
48	Intermolecular Coulombic Decay of Molecular Clusters:Â Identification of the Decay Mechanism Using a New Hole-Population Analysis. Journal of Physical Chemistry A, 1999, 103, 11145-11160.	2.5	46
49	Nuclear electric quadrupole moment of gold. Journal of Chemical Physics, 2007, 126, 064314.	3.0	46
50	Revisiting the potential energy surface for the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:mtext>He</mml:mtext><mml:mo>+</mml:mo><mml:msubsup><mml:mrow><mml:mtext>H</mml:mtext></mml:mrow><mml:mr Chemical Physics Letters, 2009, 469, 26-30.	2.6	46
51	Unraveling the Anion/Ligand Interplay in the Reaction Mechanism of Gold(I)-Catalyzed Alkoxylation of Alkynes. Organometallics, 2017, 36, 2364-2376.	2.3	45
52	Modulating the Bonding Properties of Nâ€Heterocyclic Carbenes (NHCs): A Systematic Chargeâ€Displacement Analysis. Chemistry - A European Journal, 2017, 23, 7558-7569.	3.3	45
53	Ab initioblock-Lanczos calculation of the Auger spectra ofSiF4: Strong two-hole localization effects and foreign imaging. Physical Review A, 1996, 53, 2118-2129.	2.5	44
54	Multiphoton Ionization as a clock to Reveal Molecular Dynamics with Intense Short X-ray Free Electron Laser Pulses. Physical Review Letters, 2012, 109, 263001.	7.8	44

#	Article	IF	Citations
55	Ion pairing in NHC gold(I) olefin complexes: A combined experimental/theoretical study. Journal of Organometallic Chemistry, 2010, 695, 2679-2686.	1.8	42
56	Total molecular photoionization cross-sections by algebraic diagrammatic construction-Stieltjes-Lanczos method: Benchmark calculations. Journal of Chemical Physics, 2013, 139, 144107.	3.0	42
57	Interaction components in the hydrogen halide dications. Chemical Physics Letters, 2007, 436, 322-326.	2.6	41
58	On the interatomic electronic processes following Auger decay in neon dimer. Journal of Chemical Physics, 2008, 129, 074307.	3.0	41
59	Density Relaxation in Time-Dependent Density Functional Theory: Combining Relaxed Density Natural Orbitals and Multireference Perturbation Theories for an Improved Description of Excited States. Journal of Chemical Theory and Computation, 2014, 10, 4014-4024.	5.3	41
60	Strong Electron-Donating Ligands Accelerate the Protodeauration Step in Gold(I)-Catalyzed Reactions: A Quantitative Understanding of the Ligand Effect. Organometallics, 2016, 35, 2275-2285.	2.3	41
61	A combined NMR/DFT study on the ion pair structure of [(PR¹₂R²)Au(Î·²-3-hexyne)]BF₄complexes. Dalton Transactions, 2013, 42, 4122-4131.	3.3	40
62	Hydration and alkoxylation of alkynes catalyzed by NHCâ€“Auâ€“OTf. Green Chemistry, 2018, 20, 2125-2134.	9.0	40
63	Catching the role of anisotropic electronic distribution and charge transfer in halogen bonded complexes of noble gases. Journal of Chemical Physics, 2015, 142, 184304.	3.0	39
64	Ab initiocalculation of energies and lifetimes of metastable dianions: The C22â^' resonance. Journal of Chemical Physics, 2000, 112, 6635-6642.	3.0	38
65	¹³Câ€…NMR Spectroscopy of Nâ€Heterocyclic Carbenes Can Selectively Probe Ïƒ Donation in Gold(I) Complexes. Chemistry - A European Journal, 2017, 23, 2722-2728.	3.3	38
66	On the Auger spectrum of silane. Chemical Physics Letters, 1985, 122, 169-174.	2.6	37
67	Penning ionization of N2O molecules by He*(2S3,1) and Ne*(P2,03) metastable atoms: Theoretical considerations about the intermolecular interactions. Journal of Chemical Physics, 2005, 122, 164308.	3.0	37
68	Penning ionization of N2O molecules by He*(2S3,1) and Ne*(P2,03) metastable atoms: A crossed beam study. Journal of Chemical Physics, 2005, 122, 164307.	3.0	37
69	Molecular photoionization cross sections by Stieltjesâ€“Chebyshev moment theory applied to Lanczos pseudospectra. Journal of Chemical Physics, 2009, 130, 064104.	3.0	37
70	Double vacancies in the cores of silane and tetrafluorosilane. Physical Review A, 1991, 44, 205-217.	2.5	36
71	Triple Ionization of Carbon Monoxide. Physical Review Letters, 1996, 76, 896-899.	7.8	36
72	Electron density fitting for the Coulomb problem in relativistic density-functional theory. Journal of Chemical Physics, 2006, 124, 124104.	3.0	36

#	Article	IF	Citations
73	Ionization of CH4 and some fluoromethanes: a green's function study and an (e,2e) spectroscopic investigation. Chemical Physics Letters, 1981, 80, 295-300.	2.6	35
74	Ab initiointeratomic decay widths of excited states by applying Stieltjes imaging to Lanczos pseudospectra. Journal of Chemical Physics, 2011, 134, 094107.	3.0	35
75	The Electronic Structure of Alkali Aurides. A Four-Component Diracâ^'Kohnâ^'Sham Study. Journal of Physical Chemistry A, 2006, 110, 4543-4554.	2.5	33
76	Dioxygen insertion into the gold(<scp>i</scp>)â€"hydride bond: spin orbit coupling effects in the spotlight for oxidative addition. Chemical Science, 2016, 7, 7034-7039.	7.4	33
77	Selective Emergence of the Halogen Bond in Ground and Excited States of Nobleâ€Gasâ€"Chlorine Systems. Angewandte Chemie - International Edition, 2019, 58, 4195-4199.	13.8	33
78	Ab initio calculations of the copper(2+)-O2- interaction as a model for the mechanism of copper/zinc superoxide dismutase. Inorganic Chemistry, 1986, 25, 1005-1008.	4.0	32
79	Intermolecular Coulombic decay of clusters. Journal of Electron Spectroscopy and Related Phenomena, 2001, 114-116, 41-47.	1.7	31
80	On the doubly ionized states of Ar2 and their intra- and interatomic decay to Ar23+. Journal of Chemical Physics, 2008, 128, 014307.	3.0	30
81	Nature and Stability of Weak Halogen Bonds in the Gas Phase: Molecular Beam Scattering Experiments and Ab Initio Charge Displacement Calculations. Crystal Growth and Design, 2011, 11, 4279-4283.	3.0	30
82	Theoretical study of K-shell excitations in formaldehyde. Chemical Physics, 1988, 122, 9-15.	1.9	29
83	All ab initio Auger spectra of HF and LiF: energies, intensities and vibrational shifts and broadenings. Chemical Physics Letters, 1993, 206, 247-252.	2.6	29
84	Complete valence double photoionization of SF6. Journal of Chemical Physics, 2005, 122, 144309.	3.0	29
85	Quantitative assessment of the carbocation/carbene character of the goldâ€"carbene bond. Dalton Transactions, 2015, 44, 13999-14007.	3.3	29
86	Valence ionization of HCl. An investigation of manyâ€body effects. Journal of Chemical Physics, 1990, 92, 4331-4341.	3.0	28
87	The Auger spectroscopy of pyrimidine and halogen-substituted pyrimidines. Journal of Chemical Physics, 2008, 129, 154309.	3.0	28
88	Relationship between the anion/cation relative orientation and the catalytic activity of nitrogen acyclic carbeneâ€"gold catalysts. Catalysis Science and Technology, 2015, 5, 1558-1567.	4.1	28
89	An Efficient Parallel All-Electron Four-Component Diracâ^'Kohnâ^'Sham Program Using a Distributed Matrix Approach. Journal of Chemical Theory and Computation, 2010, 6, 384-394.	5.3	27
90	Advances in Charge Displacement Analysis. Journal of Chemical Theory and Computation, 2016, 12, 1236-1244.	5.3	27

#	Article	IF	Citations
91	Dynamical core-hole screening in weak chemisorption systems. Physical Review B, 1998, 57, 7340-7351.	3.2	26
92	An experimental and theoretical study of double photoionization of CF4 using time-of-flight photoelectron-photoelectron (photoion-photoion) coincidence spectroscopy. Journal of Chemical Physics, 2006, 125, 194318.	3.0	26
93	Charge-displacement analysis for excited states. Journal of Chemical Physics, 2014, 140, 054110.	3.0	26
94	Symmetry breaking and symmetry restoring in ions of loosely bound systems. Journal of Chemical Physics, 1989, 91, 7039-7047.	3.0	25
95	Interatomic Coulombic decay and its dynamics in NeAr following K-LL Auger transition in the Ne atom. Journal of Chemical Physics, 2009, 131, .	3.0	25
96	Autoionization widths by Stieltjes imaging applied to Lanczos pseudospectra. Journal of Chemical Physics, 2011, 134, 024106.	3.0	25
97	Interaction between iron(0) and heterocumulenes: "ab initio" calculations on the model compounds Fe(CO)2(PH3)2(.eta.2-OCX) and Fe(CO)2(PH3)2(.eta.2-SCX), with X = O, S, NH, CH2. Inorganic Chemistry, 1987, 26, 3805-3811.	4.0	24
98	Total photoionization cross-sections of excited electronic states by the algebraic diagrammatic construction-Stieltjes-Lanczos method. Journal of Chemical Physics, 2014, 140, 184107.	3.0	24
99	Anomalous ligand effect in gold(i)-catalyzed intramolecular hydroamination of alkynes. Chemical Communications, 2015, 51, 5990-5993.	4.1	24
100	Helium Accepts Back-Donation In Highly Polar Complexes: New Insights into the Weak Chemical Bond. Journal of Physical Chemistry Letters, 2017, 8, 3334-3340.	4.6	24
101	Insight into the halogen-bond nature of noble gas-chlorine systems by molecular beam scattering experiments, ab initio calculations and charge displacement analysis. Physical Chemistry Chemical Physics, 2019, 21, 7330-7340.	2.8	24
102	BERTHA: Implementation of a four-component Diracâ€“Kohnâ€“Sham relativistic framework. Journal of Chemical Physics, 2020, 152, 164118.	3.0	24
103	Bonding between C2 and N2: a localization-induced .sigma. bond. Journal of the American Chemical Society, 1990, 112, 9484-9490.	13.7	23
104	Charge-Displacement Analysis of the Interaction in the Ammoniaâ€“Noble Gas Complexes. Journal of Physical Chemistry A, 2011, 115, 14657-14666.	2.5	23
105	Spinâ€Forbidden Reactions: Adiabatic Transition States Using Spinâ€“Orbit Coupled Density Functional Theory. Chemistry - A European Journal, 2018, 24, 5006-5015.	3.3	23
106	Aggregation state effects in Auger spectroscopy: The fluorineKLLspectrum of KF. Physical Review Letters, 1994, 72, 428-431.	7.8	22
107	Adiabatic and nonadiabatic effects of nuclear dynamics in spectra of decaying states: Auger spectrum of HF. Journal of Chemical Physics, 1996, 105, 9175-9181.	3.0	22
108	Subspace iteration techniques for the calculation of resonances using complex symmetric Hamiltonians. Journal of Chemical Physics, 2000, 112, 2106-2110.	3.0	22

#	Article	IF	Citations
109	H₂Oâ€“CH₄and H₂Sâ€“CH₄complexes: a direct comparison through molecular beam experiments and ab initio calculations. Physical Chemistry Chemical Physics, 2015, 17, 30613-30623.	2.8	22
110	All-electron four-component Dirac-Kohn-Sham procedure for large molecules and clusters containing heavy elements. Physical Review B, 2008, 77, .	3.2	21
111	Molecular-beam study of the ammoniaâ€“noble gas systems: Characterization of the isotropic interaction and insights into the nature of the intermolecular potential. Journal of Chemical Physics, 2011, 135, 194301.	3.0	21
112	Efficient Parallel All-Electron Four-Component Diracâ€“Kohnâ€“Sham Program Using a Distributed Matrix Approach II. Journal of Chemical Theory and Computation, 2013, 9, 5356-5364.	5.3	21
113	Full Parallel Implementation of an All-Electron Four-Component Diracâ€“Kohnâ€“Sham Program. Journal of Chemical Theory and Computation, 2014, 10, 3766-3776.	5.3	21
114	Ligand Effect on Bonding in Gold(III) Carbonyl Complexes. Inorganic Chemistry, 2018, 57, 6161-6175.	4.0	21
115	Ionization of fluoromethanes: CHF3 and CF4. A Greensì€ function study and an (e, 2e) spectroscopic investigation. Chemical Physics Letters, 1982, 90, 445-452.	2.6	20
116	Correlation phenomena in the ionization of CN dimers. Journal of Electron Spectroscopy and Related Phenomena, 1990, 51, 75-89.	1.7	20
117	Theoretical simulation of molecular Auger spectra: The carbon and oxygen KLL Auger spectra of formaldehyde. Journal of Chemical Physics, 1993, 99, 6688-6696.	3.0	20
118	The ab-initio simulation of auger spectra. Journal of Electron Spectroscopy and Related Phenomena, 1995, 76, 47-54.	1.7	20
119	The Auger spectra of CF4 in the light of foreign imaging. Journal of Chemical Physics, 1996, 104, 9754-9767.	3.0	20
120	Impact of narrow-band excitation on resonant decay spectra. Physical Review A, 1999, 60, 1079-1090.	2.5	20
121	Site-selected Auger electron spectroscopy of N2O. Journal of Chemical Physics, 2006, 125, 054306.	3.0	20
122	Interaction of O₂ with CH₄, CF₄, and CCl₄ by Molecular Beam Scattering Experiments and Theoretical Calculations. Journal of Physical Chemistry A, 2016, 120, 5197-5207.	2.5	20
123	Advances in the theoretical simulation of Auger spectra of polyatomic molecules: an example. Journal of Electron Spectroscopy and Related Phenomena, 1995, 74, 1-14.	1.7	19
124	Microsolvation of Li+in Water Analyzed by Ionization and Double Ionization. Journal of Physical Chemistry A, 2004, 108, 5831-5844.	2.5	19
125	Effects of nuclear dynamics in the low-kinetic-energy Auger spectra of CO and CO2. Journal of Chemical Physics, 2005, 123, 224306.	3.0	19
126	Computational strategies for a four-component Diracâ€“Kohnâ€“Sham program: Implementation and first applications. Journal of Chemical Physics, 2005, 122, 184109.	3.0	19

#	Article	IF	Citations
127	Poisson-transformed density fitting in relativistic four-component Diracâ€“Kohnâ€“Sham theory. Journal of Chemical Physics, 2008, 128, 124108.	3.0	19
128	The ligand effect on the oxidative addition of dioxygen to gold(<scp>i</scp>)â€“hydride complexes. Dalton Transactions, 2017, 46, 11679-11690.	3.3	19
129	Observing Femtosecond Fragmentation Using Ultrafast X-ray-Induced Auger Spectra. Applied Sciences (Switzerland), 2017, 7, 681.	2.5	19
130	Study of the interaction between iron(0) and carbon dioxide, carbonyl sulphide and carbon disulphide: â€œab initioâ€•calculations on the model compounds Fe(CO)2(PH3)2(Î·2-CO2), Fe(CO)2(PH3)2(Î·2-COS), Fe(CO)2(PH3)2(Î·2-CS2), and Fe(PH3)4(Î·2-CO2). Journal of Organometallic Chemistry, 1987, 332, 153-164.	1.8	18
131	Cyclization of 2-Alkynyldimethylaniline on Gold(I) Cationic and Neutral Complexes. Organometallics, 2016, 35, 595-604.	2.3	18
132	Alkyne Activation with Gold(III) Complexes: A Quantitative Assessment of the Ligand Effect by Charge-Displacement Analysis. Inorganic Chemistry, 2019, 58, 3115-3129.	4.0	18
133	Many-body calculation of the valence photoemission spectrum of Cr(CO)6. Physical Review B, 1992, 45, 1851-1856.	3.2	17
134	Diffusion NMR measurements on cationic linear gold(I) complexes. Polyhedron, 2015, 92, 52-59.	2.2	17
135	The Chemical Bond and sâ€“d Hybridization in Coinage Metal(I) Cyanides. Inorganic Chemistry, 2019, 58, 11716-11729.	4.0	17
136	PyBERTHART: A Relativistic Real-Time Four-Component TDDFT Implementation Using Prototyping Techniques Based on Python. Journal of Chemical Theory and Computation, 2020, 16, 2410-2429.	5.3	17
137	Leading Interaction Components in the Structure and Reactivity of Noble Gases Compounds. Molecules, 2020, 25, 2367.	3.8	17
138	Potential energy surfaces in hyperspherical coordinates: AB initio kinetic paths for the O(3P)+H2 reaction. Chemical Physics Letters, 1989, 162, 179-184.	2.6	16
139	Ab Initio Molecular Dynamics Simulations of Elimination Reactions in Water Solution:Â Exploring the Borderline Region between the E1cb and E2 Reaction Mechanisms. Journal of Physical Chemistry B, 2006, 110, 11014-11019.	2.6	16
140	Experimental strategies for optical pump â€“ soft x-ray probe experiments at the LCLS. Journal of Physics: Conference Series, 2014, 488, 012015.	0.4	16
141	The gold(<scp>iii</scp>)â€“CO bond: a missing piece in the gold carbonyl complex landscape. Chemical Communications, 2017, 53, 1603-1606.	4.1	16
142	Cooperative role of halogen and hydrogen bonding in the stabilization of water adducts with apolar molecules. New Journal of Chemistry, 2018, 42, 10603-10614.	2.8	16
143	Diisocyanogen or Isocyanogen?. Angewandte Chemie International Edition in English, 1989, 28, 761-762.	4.4	15
144	The calculation of molecular Auger spectra. Journal of Electron Spectroscopy and Related Phenomena, 1994, 68, 297-312.	1.7	15

#	Article	IF	Citations
145	Ab initio simulation of molecular Auger spectra: Nuclear dynamics effects in the spectra of carbonyl sulfide. Journal of Chemical Physics, 1997, 107, 6070-6079.	3.0	15
146	Intermolecular Interaction in the NH₃â€“H₂ and H₂Oâ€“H₂ Complexes by Molecular Beam Scattering Experiments: The Role of Charge Transfer. Journal of Physical Chemistry A, 2013, 117, 12601-12607.	2.5	15
147	Intermolecular Interaction in the H₂Sâ€“H₂ Complex: Molecular Beam Scattering Experiments and Ab-Inito Calculations. Journal of Physical Chemistry A, 2014, 118, 6440-6450.	2.5	15
148	A theoretical investigation of the copper-super-oxide system. A model for the mechanism of copper-zinc superoxide dismutase. Inorganica Chimica Acta, 1985, 107, L21-L22.	2.4	14
149	Theoretical investigations of molecular triple ionization spectra. Journal of Chemical Physics, 1996, 104, 9531-9545.	3.0	14
150	Coreâ€valence doubly ionized states: General aspects, examples, production mechanisms. Journal of Chemical Physics, 1996, 105, 11108-11133.	3.0	14
151	Parallelization of a relativistic DFT code. Future Generation Computer Systems, 2004, 20, 739-747.	7.5	14
152	An indirect approach to the determination of the nuclear quadrupole moment by four-component relativistic DFT in molecular calculations. Chemical Physics Letters, 2007, 442, 233-237.	2.6	14
153	Ultrafast Molecular Three-Electron Auger Decay. Physical Review Letters, 2016, 116, 073001.	7.8	14
154	Theoretical investigation of the energy dependence of photoionization cross-sections and angular distributions of photoemission of CH4 and CF4. Journal of Electron Spectroscopy and Related Phenomena, 1986, 41, 439-452.	1.7	13
155	Non-analyticity of self-consistent field approaches: failure of predicting symmetry. Journal of Physics B: Atomic, Molecular and Optical Physics, 1990, 23, L747-L752.	1.5	13
156	Merging of E2 and E1cb Reaction Mechanisms: A Combined Theoretical and Experimental Study. European Journal of Organic Chemistry, 2009, 2009, 5501-5504.	2.4	13
157	Resonant decay spectra for energetically unselective excitation exemplified by the broadband resonant Auger spectrum of HF. Physical Review A, 1999, 60, 1070-1078.	2.5	12
158	Local and nonlocal effects in the core ionization of metal-molecule adsorbates and cluster systems. Physical Review B, 2000, 61, 7336-7339.	3.2	12
159	On the role of charge transfer in the stabilization of weakly bound complexes involving water and hydrogen sulphide molecules. Chemical Physics, 2012, 398, 176-185.	1.9	12
160	Environmental Effects with Frozen-Density Embedding in Real-Time Time-Dependent Density Functional Theory Using Localized Basis Functions. Journal of Chemical Theory and Computation, 2020, 16, 5695-5711.	5.3	12
161	An (e, 2e) spectroscopic invistigation and a green's function study of the ionization of chloro- and bromo-ethylene. Chemical Physics Letters, 1983, 101, 477-484.	2.6	11
162	On the choice of orbital bases for configuration interaction. Journal of Chemical Physics, 1988, 89, 4170-4179.	3.0	11

#	Article	IF	Citations
163	Valence ionization and the electron affinities of the open and cyclic forms of Se3and Te3. Journal of Chemical Physics, 1989, 91, 3582-3588.	3.0	11
164	Foreign and native coordination effects in core-level spectra of mixed Be-Mg clusters. Journal of Chemical Physics, 2002, 117, 3533-3536.	3.0	11
165	Theoretical investigation of the ground and core hole states of [Cu(NH3)2CO]+ and [Cu(NH3)3CO]+. Models for the reversible binding of carbon monoxide to copper(I) complexes. Inorganic Chemistry, 1981, 20, 2602-2607.	4.0	10
166	Benchmarking a model potential for the investigation of intermolecular interactions. Physica Scripta, 2008, 78, 038102.	2.5	10
167	Modelling Charge Transfer in Weak Chemical Bonds: Insights from the Chemistry of Helium. ChemPhysChem, 2018, 19, 1476-1485.	2.1	10
168	An (e, 2e) spectroscopic investigation and a Green's function study of the ionization of fluoroethylene. Molecular Physics, 1982, 45, 839-852.	1.7	9
169	A theoretical study on the co-ordination of dinitrogen and related molecules to nickel(0): â€˜ab initioâ€™ calculations on the model compounds [Ni(PH3)2(N2)], [Ni(PH3)2(N2CH2)], and [Ni(PH3)2(N2H2)]. Journal of the Chemical Society Dalton Transactions, 1989, , 33-38.	1.1	9
170	The ab initio calculation of very many triply ionized states of molecular systems. Journal of Electron Spectroscopy and Related Phenomena, 1995, 75, 109-115.	1.7	9
171	Strong charge-transfer effects in the Mg2pâ^'1core-level spectrum ofMgB2. Physical Review B, 2002, 66, .	3.2	9
172	Double ionization of fluorinated benzenes: Hole localization and delocalization effects. Journal of Chemical Physics, 2004, 120, 1775-1791.	3.0	9
173	Implementation and use of a direct, partially integralâ€driven nonâ€Dyson propagator method for molecular ionization. Journal of Computational Chemistry, 2009, 30, 818-825.	3.3	9
174	Anab initioelectronic density study of the CH₄â€“Ar, CH₄â€“Xe, CH₄â€“H₂O and CH₄â€“H₂S complexes: insights into the nature of the intermolecular interaction. Molecular Physics, 2015, 113, 3992-3999.	1.7	9
175	A non-empirical LCAO MO SCF investigation of the ground and core hole states of some simple AH2 systems. Chemical Physics, 1980, 52, 1-9.	1.9	8
176	Interaction between iron(0) and formaldehyde, thioformaldehyde, and acetone: ab initio calculations on the model compounds Fe(CO)2(PH3)2(.eta.2-CH2O), Fe(CO)2(PH3)2(.eta.2-CH2S), Fe(PH3)4(.eta.2-CH2O), and Fe(PH3)4(.eta.2-CMe2O). Inorganic Chemistry, 1988, 27, 69-73.	4.0	8
177	On the auger spectrum of ethylene. Journal of Electron Spectroscopy and Related Phenomena, 1990, 51, 211-219.	1.7	8
178	Linear Algebra Computation Benchmarks on a Model Grid Platform. Lecture Notes in Computer Science, 2003, , 297-306.	1.3	8
179	An XÎ± Investigation of Photoelectron Spectra and Bond Structure of Fluorides and Oxyfluorides of Nitrogen and Phosphorus. Zeitschrift Fur Physikalische Chemie, 1981, 127, 1-12.	2.8	7
180	A CI investigation on the core ionized and core-Rydberg excited states of NH2. Chemical Physics Letters, 1982, 91, 178-184.	2.6	7

#	Article	IF	Citations
181	Orbital coupling in double-vacancy and two-electron systems. Chemical Physics Letters, 1991, 183, 1-8.	2.6	7
182	Partial localization of core holes in nonsymmetrical systems. Physical Review B, 1998, 58, 2316-2323.	3.2	7
183	Valence-hole localization in core-valence doubly ionized states of ionic molecules and its impact onKLVAuger spectroscopy. Physical Review A, 1999, 60, 2047-2062.	2.5	7
184	Double photoionization of thiophene and bromine-substituted thiophenes. Journal of Chemical Physics, 2008, 129, 234303.	3.0	7
185	A CI investigation of the core ionized states derived from 1A1 and 3B1 methylene. Chemical Physics, 1980, 52, 11-21.	1.9	6
186	Non-Hartree-Fock mean fields for molecules: critical tests. Journal of Physics B: Atomic and Molecular Physics, 1987, 20, 5259-5265.	1.6	6
187	X? SW studies on C ls level photoionization cross sections and angular distributions for fluoromethanes. Journal of Structural Chemistry, 1989, 30, 147-148.	1.0	6
188	Core hole screening in chemisorption systems: Role of metal-adsorbate Ï€â†'Ï€* charge transfer. Physical Review B, 1996, 54, 10405-10408.	3.2	6
189	Theory of wave packet dynamics: resonant Auger spectrum of HF. Journal of Electron Spectroscopy and Related Phenomena, 1998, 93, 17-30.	1.7	6
190	The Halogen-Bond Nature in Noble Gasâ€"Dihalogen Complexes from Scattering Experiments and Ab Initio Calculations. Molecules, 2019, 24, 4274.	3.8	6
191	Halogen bond interaction: Role of hybridization and induction. Chemical Physics Letters, 2021, 771, 138522.	2.6	6
192	A CI investigation on the ionized states of BeH2. Chemical Physics Letters, 1981, 83, 320-323.	2.6	5
193	Ionization of fluorinated methanes and ethylenes through (e,2e) process and green's function approach to predict ionization potentials. International Journal of Mass Spectrometry and Ion Physics, 1983, 46, 261-264.	1.3	5
194	Calculating triply ionized states of molecules by Green's functions: carbon monoxide. Journal of Electron Spectroscopy and Related Phenomena, 1995, 76, 307-312.	1.7	5
195	On the calculation of shake-off satellite contributions to molecular Auger spectra. Chemical Physics Letters, 1996, 251, 26-32.	2.6	5
196	A DFT investigation of base-catalyzed Î²-elimination reactions in water solution for systems activated by the pyridine ring: Theory vs. experiment. Chemical Physics Letters, 2008, 460, 100-107.	2.6	5
197	Radiationless decay in the region of the 2t2g and 4eg resonances in SF6. Journal of Chemical Physics, 2011, 134, 094308.	3.0	5
198	Sequential multiple ionization and fragmentation of SF6induced by an intense free electron laser pulse. Journal of Physics B: Atomic, Molecular and Optical Physics, 2013, 46, 164032.	1.5	5

#	Article	IF	Citations
199	[illegible] electron solvation in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si6.gif" overflow="scroll"><mml:msup><mml:mi mathvariant="normal">Li</mml:mi><mml:mo>â^</mml:mo></mml:msup><mml:msub><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:msub><mml:mi) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 737 Td (mathvariant="normal">NH	2.6	5
200	Epidemiological studies ofPseudomonas aeruginosa infections in leg ulcers. Medical Microbiology and Immunology, 1983, 172, 41-45.	4.8	4
201	Ironâ€“formaldehyde interaction: â€˜ab initioâ€™ calculations on the model compounds [Fe(CO)4â€“n(PH3)n(Î·2-CH2O)](n= 0, 2, or 4). Journal of the Chemical Society Dalton Transactions, 1988, , 321-327.	1.1	4
202	A photoelectron and double photoionization study of the valence electronic structure of 1,4-bromofluorobenzene. Journal of Chemical Physics, 2009, 131, 184302.	3.0	4
203	DFT studies of Î²-elimination reactions in water solution with different bases: Theory vs experiment. Computational and Theoretical Chemistry, 2010, 940, 103-114.	1.5	4
204	Chemical Bond Mechanism for Helium Revealed by Electronic Excitation. Journal of Physical Chemistry A, 2019, 123, 6572-6577.	2.5	4
205	Selective Emergence of the Halogen Bond in Ground and Excited States of Nobleâ€Gasâ€“Chlorine Systems. Angewandte Chemie, 2019, 131, 4239-4243.	2.0	4
206	Orbital Decomposition of the Carbon Chemical Shielding Tensor in Gold(I) Nâ€Heterocyclic Carbene Complexes. European Journal of Inorganic Chemistry, 2020, 2020, 1177-1183.	2.0	4
207	Study of relative stabilities of the intermediates in catalytic carbon monoxide hydrogenation reactions: ab initio calculations on the model compounds [Fe(CO)2(PH3)2H2], [Fe(CO)2(PH3)2(CHO)H], [Fe(CO)2(PH3)2(CH2O)], and [Fe(CO)(PH3)2(CHO)2]. Journal of the Chemical Society Dalton Transactions, 1988, , 249.	1.1	3
208	Relativistic quantum chemistry involving heavy atoms. Rendiconti Lincei, 2018, 29, 209-217.	2.2	3
209	An experimental ESCA investigation of some copper complexes involving CO. Inorganica Chimica Acta, 1984, 87, 67-69.	2.4	2
210	Study of the interaction between iron(0) and dinitrogen: â€œab initioâ€•calculations on the model compound Fe(PH3)4(N2). Journal of Organometallic Chemistry, 1988, 348, C27-C32.	1.8	2
211	Theoretical Evidence for Delocalized Inequivalent Core Holes. Journal of Physical Chemistry A, 1998, 102, 9405-9409.	2.5	2
212	Green's function calculations for doubly ionized molecular states and simulation of Auger spectra. Canadian Journal of Physics, 1996, 74, 789-803.	1.1	1
213	Strong dynamical screening in weak chemisorption systems. Surface Science, 1998, 402-404, 508-512.	1.9	1
214	Probing nucleobase photoprotection with soft x-rays. EPJ Web of Conferences, 2013, 41, 07004.	0.3	1
215	Charge Transfer in Beryllium Bonds and Cooperativity of Beryllium and Halogen Bonds. A New Perspective. Challenges and Advances in Computational Chemistry and Physics, 2016, , 461-489.	0.6	1
216	Theoretical study of fluoromethane photoionization cross sections and angular distributions. Journal of Structural Chemistry, 1989, 30, 66-71.	1.0	0

#	Article	IF	Citations
217	On core-hole screening in chemisorption systems. Surface Science, 1997, 377-379, 623-628.	1.9	0
218	Multiple Ionization and Double Core-Hole Production in Molecules using the LCLS X-Ray FEL. Journal of Physics: Conference Series, 2012, 388, 032028.	0.4	0
219	X-Ray FEL-induced Double Core-Hole Formation in Polyatomic Molecules. Journal of Physics: Conference Series, 2012, 388, 022083.	0.4	0
220	Three-electron collective Auger decay in CH3F. Journal of Physics: Conference Series, 2015, 635, 112031.	0.4	0
221	Frontispiece: Spin-Forbidden Reactions: Adiabatic Transition States Using Spin-Orbit Coupled Density Functional Theory. Chemistry - A European Journal, 2018, 24, .	3.3	0