Francesco Tarantelli

List of Publications by Year
in descending order

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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	Halogen bond interaction: Role of hybridization and induction. Chemical Physics Letters, 2021, 771, 138522.	2.6	6
2	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
3	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
4	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
5	BERTHA: Implementation of a four-component Diracâ€“Kohnâ€“Sham relativistic framework. Journal of Chemical Physics, 2020, 152, 164118.	3.0	24
6	Leading Interaction Components in the Structure and Reactivity of Noble Gases Compounds. Molecules, 2020, 25, 2367.	3.8	17
7	The Chemical Bond and sâ€“d Hybridization in Coinage Metal(I) Cyanides. Inorganic Chemistry, 2019, 58, 11716-11729.	4.0	17
8	Chemical Bond Mechanism for Helium Revealed by Electronic Excitation. Journal of Physical Chemistry A, 2019, 123, 6572-6577.	2.5	4
9	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
10	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
11	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
12	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
13	The Halogen-Bond Nature in Noble Gasâ€“Dihalogen Complexes from Scattering Experiments and Ab Initio Calculations. Molecules, 2019, 24, 4274.	3.8	6
14	Hydration and alkoxylation of alkynes catalyzed by NHCâ€“Auâ€“OTf. Green Chemistry, 2018, 20, 2125-2134.	9.0	40
15	Modelling Charge Transfer in Weak Chemical Bonds: Insights from the Chemistry of Helium. ChemPhysChem, 2018, 19, 1476-1485.	2.1	10
16	Frontispiece: Spin-Forbidden Reactions: Adiabatic Transition States Using Spin-Orbit Coupled Density Functional Theory. Chemistry - A European Journal, 2018, 24, .	3.3	0
17	Relativistic quantum chemistry involving heavy atoms. Rendiconti Lincei, 2018, 29, 209-217.	2.2	3
18	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

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19	Spinâ€Forbidden Reactions: Adiabatic Transition States Using Spinâ€“Orbit Coupled Density Functional Theory. Chemistry - A European Journal, 2018, 24, 5006-5015.	3.3	23
20	Ligand Effect on Bonding in Gold(III) Carbonyl Complexes. Inorganic Chemistry, 2018, 57, 6161-6175.	4.0	21
21	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
22	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
23	Unraveling the Anion/Ligand Interplay in the Reaction Mechanism of Gold(I)-Catalyzed Alkoxylation of Alkynes. Organometallics, 2017, 36, 2364-2376.	2.3	45
24	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
25	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
26	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
27	Observing Femtosecond Fragmentation Using Ultrafast X-ray-Induced Auger Spectra. Applied Sciences (Switzerland), 2017, 7, 681.	2.5	19
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	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
30	Ï€ Activation of Alkynes in Homogeneous and Heterogeneous Gold Catalysis. Journal of Physical Chemistry A, 2016, 120, 5239-5247.	2.5	49
31	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
32	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
33	Ultrafast Molecular Three-Electron Auger Decay. Physical Review Letters, 2016, 116, 073001.	7.8	14
34	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
35	Advances in Charge Displacement Analysis. Journal of Chemical Theory and Computation, 2016, 12, 1236-1244.	5.3	27
36	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

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37	Cyclization of 2-Alkynyldimethylaniline on Gold(I) Cationic and Neutral Complexes. Organometallics, 2016, 35, 595-604.	2.3	18
38	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
39	Selectively Measuring Ï€â€…Backâ€Donation in Gold(I) Complexes by NMR Spectroscopy. Chemistry - A European Journal, 2015, 21, 2467-2473.	3.3	53
40	Three-electron collective Auger decay in CH3F. Journal of Physics: Conference Series, 2015, 635, 112031.	0.4	0
41	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
42	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
43	Anomalous ligand effect in gold(i)-catalyzed intramolecular hydroamination of alkynes. Chemical Communications, 2015, 51, 5990-5993.	4.1	24
44	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
45	Quantitative assessment of the carbocation/carbene character of the goldâ€“carbene bond. Dalton Transactions, 2015, 44, 13999-14007.	3.3	29
46	Diffusion NMR measurements on cationic linear gold(I) complexes. Polyhedron, 2015, 92, 52-59.	2.2	17
47	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
48	Tracing 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 ETQq0 0 0 rgBT /Overlock 10 Tf 50 297 Td (mathvariant="normal">NH</mml:mi>	2.6	5
49	H₂Oâ€“CH₄ and H₂Sâ€“CH₄ complexes: a direct comparison through molecular beam experiments and ab initio calculations. Physical Chemistry Chemical Physics, 2015, 17, 30613-30623.	2.8	22
50	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
51	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
52	Charge-displacement analysis for excited states. Journal of Chemical Physics, 2014, 140, 054110.	3.0	26
53	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
54	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

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55	The Chemical Bond in Gold(I) Complexes with N-Heterocyclic Carbenes. Organometallics, 2014, 33, 4200-4208.	2.3	73
56	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
57	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
58	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
59	A Quantitative View of Charge Transfer in the Hydrogen Bond: The Water Dimer Case. ChemPhysChem, 2014, 15, 2682-2687.	2.1	55
60	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
61	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
62	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
63	NHC-Gold-Alkyne Complexes: Influence of the Carbene Backbone on the Ion Pair Structure. Organometallics, 2013, 32, 4444-4447.	2.3	56
64	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
65	Total molecular photoionization cross-sections by algebraic diagrammatic construction-Stieltjes-Lanczos method: Benchmark calculations. Journal of Chemical Physics, 2013, 139, 144107.	3.0	42
66	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
67	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
68	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
69	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
70	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
71	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
72	Probing nucleobase photoprotection with soft x-rays. EPJ Web of Conferences, 2013, 41, 07004.	0.3	1

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73	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
74	X-Ray FEL-induced Double Core-Hole Formation in Polyatomic Molecules. Journal of Physics: Conference Series, 2012, 388, 022083.	0.4	0
75	Revealing Charge-Transfer Effects in Gas-Phase Water Chemistry. Accounts of Chemical Research, 2012, 45, 1571-1580.	15.6	107
76	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
77	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
78	Recent advances and perspectives in four-component Diracâ€“Kohnâ€“Sham calculations. Physical Chemistry Chemical Physics, 2011, 13, 12368.	2.8	59
79	Charge-Displacement Analysis of the Interaction in the Ammoniaâ€“Noble Gas Complexes. Journal of Physical Chemistry A, 2011, 115, 14657-14666.	2.5	23
80	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
81	Ab initiointeratomic decay widths of excited states by applying Stieltjes imaging to Lanczos pseudospectra. Journal of Chemical Physics, 2011, 134, 094107.	3.0	35
82	Radiationless decay in the region of the 2t2g and 4eg resonances in SF6. Journal of Chemical Physics, 2011, 134, 094308.	3.0	5
83	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
84	Autoionization widths by Stieltjes imaging applied to Lanczos pseudospectra. Journal of Chemical Physics, 2011, 134, 024106.	3.0	25
85	On the Dewarâ€“Chattâ€“Duncanson Model for Catalytic Gold(I) Complexes. Chemistry - A European Journal, 2010, 16, 7231-7240.	3.3	91
86	Ion pairing in NHC gold(I) olefin complexes: A combined experimental/theoretical study. Journal of Organometallic Chemistry, 2010, 695, 2679-2686.	1.8	42
87	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
88	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
89	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
90	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

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91	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
92	Auger Electron Angular Distribution of Double Core-Hole States in the Molecular Reference Frame. Physical Review Letters, 2010, 105, 083004.	7.8	163
93	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
94	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
95	Molecular photoionization cross sections by Stieltjesâ€“Chebyshev moment theory applied to Lanczos pseudospectra. Journal of Chemical Physics, 2009, 130, 064104.	3.0	37
96	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
97	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
98	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
99	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> Chemical Physics Letters, 2009, 469, 26-30.	2.6	46
100	Ion Pairing in Cationic Olefinâ˜Gold(I) Complexes. Journal of the American Chemical Society, 2009, 131, 3170-3171.	13.7	134
101	Experimental and theoretical evidence of charge transfer in weakly bound complexes of water. Physical Chemistry Chemical Physics, 2009, 11, 9970.	2.8	52
102	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
103	Benchmarking a model potential for the investigation of intermolecular interactions. Physica Scripta, 2008, 78, 038102.	2.5	10
104	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
105	The Auger spectroscopy of pyrimidine and halogen-substituted pyrimidines. Journal of Chemical Physics, 2008, 129, 154309.	3.0	28
106	Poisson-transformed density fitting in relativistic four-component Diracâ€“Kohnâ€“Sham theory. Journal of Chemical Physics, 2008, 128, 124108.	3.0	19
107	Double photoionization of thiophene and bromine-substituted thiophenes. Journal of Chemical Physics, 2008, 129, 234303.	3.0	7
108	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

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109	On the interatomic electronic processes following Auger decay in neon dimer. Journal of Chemical Physics, 2008, 129, 074307.	3.0	41
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	Nuclear electric quadrupole moment of gold. Journal of Chemical Physics, 2007, 126, 064314.	3.0	46
112	Interaction components in the hydrogen halide dications. Chemical Physics Letters, 2007, 436, 322-326.	2.6	41
113	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
114	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
115	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
116	The calculation of molecular double ionization spectra by Greenâ€™s functions. Chemical Physics, 2006, 329, 11-21.	1.9	49
117	Site-selected Auger electron spectroscopy of N2O. Journal of Chemical Physics, 2006, 125, 054306.	3.0	20
118	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
119	Electron density fitting for the Coulomb problem in relativistic density-functional theory. Journal of Chemical Physics, 2006, 124, 124104.	3.0	36
120	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
121	Complete valence double photoionization of SF6. Journal of Chemical Physics, 2005, 122, 144309.	3.0	29
122	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
123	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
124	Computational strategies for a four-component Diracâ€“Kohnâ€“Sham program: Implementation and first applications. Journal of Chemical Physics, 2005, 122, 184109.	3.0	19
125	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
126	Double ionization of fluorinated benzenes: Hole localization and delocalization effects. Journal of Chemical Physics, 2004, 120, 1775-1791.	3.0	9

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127	Parallelization of a relativistic DFT code. Future Generation Computer Systems, 2004, 20, 739-747.	7.5	14
128	Microsolvation of Li+in Water Analyzed by Ionization and Double Ionization. Journal of Physical Chemistry A, 2004, 108, 5831-5844.	2.5	19
129	Linear Algebra Computation Benchmarks on a Model Grid Platform. Lecture Notes in Computer Science, 2003, , 297-306.	1.3	8
130	Strong charge-transfer effects in the Mg2pâ^'1core-level spectrum ofMgB2. Physical Review B, 2002, 66, .	3.2	9
131	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
132	Intermolecular Coulombic decay of clusters. Journal of Electron Spectroscopy and Related Phenomena, 2001, 114-116, 41-47.	1.7	31
133	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
134	Subspace iteration techniques for the calculation of resonances using complex symmetric Hamiltonians. Journal of Chemical Physics, 2000, 112, 2106-2110.	3.0	22
135	Ab initiocalculation of energies and lifetimes of metastable dianions: The C22â^' resonance. Journal of Chemical Physics, 2000, 112, 6635-6642.	3.0	38
136	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
137	Impact of narrow-band excitation on resonant decay spectra. Physical Review A, 1999, 60, 1079-1090.	2.5	20
138	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
139	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
140	Theory of wave packet dynamics: resonant Auger spectrum of HF. Journal of Electron Spectroscopy and Related Phenomena, 1998, 93, 17-30.	1.7	6
141	Strong dynamical screening in weak chemisorption systems. Surface Science, 1998, 402-404, 508-512.	1.9	1
142	Theoretical Evidence for Delocalized Inequivalent Core Holes. Journal of Physical Chemistry A, 1998, 102, 9405-9409.	2.5	2
143	Highly excited electronic states of molecular clusters and their decay. Journal of Chemical Physics, 1998, 108, 9737-9750.	3.0	60
144	Controlled Interplay between Decay and Fragmentation in Resonant Auger Processes. Physical Review Letters, 1998, 80, 1865-1868.	7.8	48

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145	Partial localization of core holes in nonsymmetrical systems. Physical Review B, 1998, 58, 2316-2323.	3.2	7
146	Dynamical core-hole screening in weak chemisorption systems. Physical Review B, 1998, 57, 7340-7351.	3.2	26
147	Giant Intermolecular Decay and Fragmentation of Clusters. Physical Review Letters, 1997, 79, 4778-4781.	7.8	634
148	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
149	On core-hole screening in chemisorption systems. Surface Science, 1997, 377-379, 623-628.	1.9	0
150	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
151	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
152	On the calculation of shake-off satellite contributions to molecular Auger spectra. Chemical Physics Letters, 1996, 251, 26-32.	2.6	5
153	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
154	Theoretical investigations of molecular triple ionization spectra. Journal of Chemical Physics, 1996, 104, 9531-9545.	3.0	14
155	Coreâ€valence doubly ionized states: General aspects, examples, production mechanisms. Journal of Chemical Physics, 1996, 105, 11108-11133.	3.0	14
156	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
157	The Auger spectra of CF4 in the light of foreign imaging. Journal of Chemical Physics, 1996, 104, 9754-9767.	3.0	20
158	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
159	Triple Ionization of Carbon Monoxide. Physical Review Letters, 1996, 76, 896-899.	7.8	36
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