Mauro Stener

List of Publications by Year
in descending order

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206 papers	5,672 citations	61857 43 h-index	118652 62 g-index
209 all docs	209 docs citations	209 times ranked	4516 citing authors

#	Article	IF	Citations
1	From clusters to bulk: A relativistic density functional investigation on a series of gold clusters Aun, n=6,â€¦,147. Journal of Chemical Physics, 1997, 106, 5189-5201.	1.2	340
2	Time dependent density functional theory of core electrons excitations. Chemical Physics Letters, 2003, 373, 115-123.	1.2	232
3	Au₂₄(SAdm)₁₆ Nanomolecules: X-ray Crystal Structure, Theoretical Analysis, Adaptability of Adamantane Ligands to Form Au₂₃(SAdm)₁₆ and Au₂₅(SAdm)₁₆, and Its Relation to Au₂₅(SR)₁₈. Journal of the American Chemical Society, 2014, 136, 14933-14940.	6.6	139
4	Convergence of the multicenter B-spline DFT approach for the continuum. Chemical Physics, 2002, 276, 25-43.	0.9	129
5	Density Functional Study on the Morphology and Photoabsorption of CdSe Nanoclusters. Journal of Physical Chemistry C, 2011, 115, 16782-16796.	1.5	104
6	Optical Properties of Au Nanoclusters from TD-DFT Calculations. Journal of Physical Chemistry C, 2011, 115, 6277-6282.	1.5	100
7	Time-dependent density-functional theory for molecular photoionization with noniterative algorithm and multicenter B-spline basis set: CS2 and C6H6 case studies. Journal of Chemical Physics, 2005, 122, 234301.	1.2	91
8	Valence photoionization dynamics in circular dichroism of chiral free molecules: The methyl-oxirane. Journal of Chemical Physics, 2005, 122, 244303.	1.2	89
9	Circular dichroism in photoelectron spectroscopy of free chiral molecules: Experiment and theory on methyl-oxirane. Physical Review A, 2004, 70, .	1.0	78
10	Femtosecond photoelectron diffraction on laser-aligned molecules: Towards time-resolved imaging of molecular structure. Physical Review A, 2013, 88, .	1.0	76
11	Density functional study on the circular dichroism of photoelectron angular distribution from chiral derivatives of oxirane. Journal of Chemical Physics, 2004, 120, 3284-3296.	1.2	74
12	Crystal Structure and Theoretical Analysis of Green Gold Au₃₀(S-tBu)₁₈ Nanomolecules and Their Relation to Au₃₀S(S-tBu)₁₈. Journal of Physical Chemistry C, 2016, 120, 6256-6261.	1.5	72
13	Density functional-time-dependent local density approximation calculations of autoionization resonances in noble gases. Journal of Physics B: Atomic, Molecular and Optical Physics, 1995, 28, 4973-4999.	0.6	68
14	NaxAu and CsxAu bimetal clusters: Finite size analogs of sodiumâ€“gold and cesiumâ€“gold compounds. Journal of Chemical Physics, 1996, 105, 5574-5585.	1.2	67
15	Time-dependent density functional calculations of molecular photoionization cross sections: N2 and PH3. Journal of Chemical Physics, 2000, 112, 10871-10879.	1.2	66
16	Au₂₇₉(SR)₈₄: The Smallest Gold Thiolate Nanocrystal That Is Metallic and the Birth of Plasmon. Journal of Physical Chemistry Letters, 2018, 9, 1295-1300.	2.1	65
17	Alloying Effects on the Optical Properties of Agâ€“Au Nanoclusters from TDDFT Calculations. Journal of Physical Chemistry C, 2011, 115, 24085-24091.	1.5	61
18	Density functional calculations of excitation energies and oscillator strengths for and excitations and ionization potentials in carbonyl containing molecules. Chemical Physics, 1995, 191, 141-154.	0.9	60

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19	Gold Nanowires: A Time-Dependent Density Functional Assessment of Plasmonic Behavior. Journal of Physical Chemistry C, 2013, 117, 17196-17204.	1.5	60
20	Spinâ€“orbit relativistic time dependent density functional theory calculations for the description of core electron excitations: TiCl4 case study. Chemical Physics Letters, 2005, 416, 56-63.	1.2	59
21	Selecting core-hole localization or delocalization in CS2 by photofragmentation dynamics. Nature Communications, 2015, 6, 6166.	5.8	59
22	Transformation of Au₁₄₄(SCH₂CH₂Ph)₆₀ to Au₁₃₃(SPh-tBu)₅₂ Nanomolecules: Theoretical and Experimental Study. Journal of Physical Chemistry Letters, 2015, 6, 2134-2139.	2.1	58
23	Theoretical study of resonances in the metal core photoionization of M@C60(M = Li, Na, K). Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 4523-4534.	0.6	57
24	Photoabsorption of Icosahedral Noble Metal Clusters: An Efficient TDDFT Approach to Large-Scale Systems. Journal of Physical Chemistry C, 2016, 120, 12773-12782.	1.5	57
25	Long-Lived Palladium Catalysts for CO/Vinyl Arene Polyketones Synthesis: A Solution to Deactivation Problems. Chemistry - A European Journal, 2006, 12, 7639-7651.	1.7	56
26	Chiral Functionalization of an Atomically Precise Noble Metal Cluster: Insights into the Origin of Chirality and Photoluminescence. ACS Nano, 2020, 14, 9687-9700.	7.3	56
27	Valence photoionization of C6H6 by the B-spline one-centre expansion density functional method. Chemical Physics, 1998, 234, 95-109.	0.9	55
28	Imaging molecular structure through femtosecond photoelectron diffraction on aligned and oriented gas-phase molecules. Faraday Discussions, 2014, 171, 57-80.	1.6	55
29	Density functional calculations of photoionization with an exchange-correlation potential with the correct asymptotic behaviour. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 1081-1102.	0.6	53
30	Time dependent density functional photoionization of CH4, NH3, H2O and HF. Chemical Physics, 2002, 282, 337-351.	0.9	48
31	X-ray Absorption Spectroscopy of Titanium Oxide by Time Dependent Density Functional Calculations. Journal of Physical Chemistry B, 2006, 110, 9899-9907.	1.2	48
32	Self-Assembled Metallacycles with Pyrazine Edges:â€‰ A New Example in Which the Unexpected Molecular Triangle Prevails over the Expected Molecular Square. Inorganic Chemistry, 2007, 46, 11243-11253.	1.9	48
33	The Missing Link: Au191(SPh-tBu)66 Janus Nanoparticle with Molecular and Bulk-Metal-like Properties. Journal of the American Chemical Society, 2020, 142, 15799-15814.	6.6	48
34	Vibrationally resolved high-resolution NEXAFS and XPS spectra of phenanthrene and coronene. Journal of Chemical Physics, 2014, 141, 044313.	1.2	47
35	Conformational Effects on Circular Dichroism in the Photoelectron Angular Distribution. ChemPhysChem, 2006, 7, 924-934.	1.0	46
36	A study of the valence shell electronic states of pyrimidine and pyrazine by photoabsorption spectroscopy and time-dependent density functional theory calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 075203.	0.6	46

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37	Resonant Circular Dichroism of Chiral Metal-Organic Complex. Physical Review Letters, 2012, 108, 083001.	2.9	46
38	Femtosecond x-ray photoelectron diffraction on gas-phase dibromobenzene molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 124035.	0.6	46
39	Conformational Effects in Photoelectron Circular Dichroism of Alaninol. ChemPhysChem, 2009, 10, 1839-1846.	1.0	45
40	A new time dependent density functional algorithm for large systems and plasmons in metal clusters. Journal of Chemical Physics, 2015, 143, 024106.	1.2	45
41	Optical properties of nanoalloys. Physical Chemistry Chemical Physics, 2015, 17, 27952-27967.	1.3	45
42	Photoionization of C60 by large scale one-center density functional explicit continuum wave-function. Journal of Chemical Physics, 1999, 111, 4589-4597.	1.2	44
43	Complexed bridging ligands: oxorhenium(V) compounds with mono-coordinated pyrazine or pyrimidine as possible building blocks for the construction of polynuclear architecturesâ€Šâ€. Dalton Transactions RSC, 2001, , 1338-1346.	2.3	44
44	2p x-ray absorption spectroscopy of 3d transition metal systems. Journal of Electron Spectroscopy and Related Phenomena, 2021, 249, 147061.	0.8	44
45	Theoretical study on the circular dichroism in core and valence photoelectron angular distributions of camphor enantiomers. Journal of Chemical Physics, 2006, 124, 024326.	1.2	41
46	Decay Channel Dependence of the Photoelectron Angular Distributions in Core-Level Ionization of Ne Dimers. Physical Review Letters, 2008, 101, 043004.	2.9	40
47	Multidimensional calculation of time-resolved photoelectron angular distributions: The internal conversion dynamics of pyrazine. Journal of Chemical Physics, 2003, 118, 4432-4443.	1.2	38
48	Palladium Complexes with 3-Alkyl-Substituted-1,10-Phenanthrolines:â€‰ Effect of the Remote Alkyl Substituent on the CO/Olefin Copolymerization Reactions. Organometallics, 2004, 23, 5593-5605.	1.1	38
49	Theoretical Study of Near-Edge X-ray Absorption Fine Structure Spectra of Metal Phthalocyanines at C and N K-Edges. Journal of Physical Chemistry A, 2012, 116, 2885-2894.	1.1	38
50	Optical Properties of Silver Nanoshells from Time-Dependent Density Functional Theory Calculations. Journal of Physical Chemistry C, 2014, 118, 12450-12458.	1.5	38
51	Theoretical study of the valence and core photoemission spectra of C60. Physical Chemistry Chemical Physics, 2001, 3, 4481-4487.	1.3	36
52	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.	1.0	36
53	A study of the valence shell photoionisation dynamics of pyrimidine and pyrazine. Chemical Physics, 2011, 390, 25-35.	0.9	36
54	Density functional study of structural properties and binding energies of dimethylsulfoxide Ru(II) complexes. Computational and Theoretical Chemistry, 2000, 497, 91-104.	1.5	35

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55	Optical Excitations of Gold Nanoparticles:â€‰ A Quantum Chemical Scalar Relativistic Time Dependent Density Functional Study. Journal of Physical Chemistry C, 2007, 111, 11862-11871.	1.5	35
56	Conformational Sensitivity in Photoelectron Circular Dichroism of 3â€Methylcyclopentanone. ChemPhysChem, 2013, 14, 1723-1732.	1.0	35
57	Recent advances in molecular photoionization by density functional theory based approaches. Theoretical Chemistry Accounts, 2007, 117, 943-956.	0.5	34
58	Molecular orbital description of core excitation spectra in transition metal compounds. An ab initio CI calcultaion on TiCl4 and isoelectronic molecules. Chemical Physics, 1994, 186, 1-16.	0.9	33
59	Valence and core photoemission in M@C60(M = Be, Mg, Ca). Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 1421-1438.	0.6	33
60	Angle-Resolved Photoelectron Spectroscopy of Randomly Oriented 3-Hydroxytetrahydrofuran Enantiomers. ChemPhysChem, 2005, 6, 1164-1168.	1.0	33
61	3D mapping of photoemission from a single oriented H₂O molecule. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 051001.	0.6	33
62	Au₃₈(SPh)₂₄: Au₃₈ Protected with Aromatic Thiolate Ligands. Journal of Physical Chemistry Letters, 2017, 8, 1530-1537.	2.1	33
63	Designing ligand-enhanced optical absorption of thiolated gold nanoclusters. Chemical Communications, 2015, 51, 7935-7938.	2.2	31
64	High energy oscillations in the valence photoionization partial cross-section of C60. Chemical Physics Letters, 2001, 348, 363-367.	1.2	30
65	Time Dependent Density Functional Theory of X-ray Absorption Spectroscopy of Alkaline-Earth Oxides. Journal of Physical Chemistry B, 2005, 109, 10332-10340.	1.2	30
66	X-ray Absorption Spectroscopy of VOCl3, CrO2Cl2, and MnO3Cl: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 2914-2925.	1.1	30
67	Atomically precise Au₁₄₄(SR)₆₀ nanoclusters (R = Et, Pr) are capped by 12 distinct ligand types of 5-fold equivalence and display gigantic diastereotopic effects. Chemical Science, 2018, 9, 8796-8805.	3.7	30
68	Au₂₁S(SAdm)₁₅: Crystal Structure, Mass Spectrometry, Optical Spectroscopy, and First-Principles Theoretical Analysis. Journal of Physical Chemistry C, 2017, 121, 10865-10869.	1.5	29
69	Time dependent density functional study of the photoionization dynamics of SF6. Journal of Chemical Physics, 2006, 124, 114306.	1.2	28
70	Principles of Optical Spectroscopy of Aromatic Alloy Nanomolecules: Au_{36â€“x}Ag_x(SPh-tBu)₂₄. Journal of Physical Chemistry C, 2018, 122, 4524-4531.	1.5	28
71	Time dependent density functional study of the symmetry resolved N 1s photoionization in N2. Chemical Physics Letters, 2002, 351, 469-474.	1.2	27
72	Time-Dependent Density Functional Theory Calculations of Ligand K Edge and Metal L Edge X-ray Absorption of a Series of Oxomolybdenum Complexes. Journal of Physical Chemistry A, 2004, 108, 8467-8477.	1.1	27

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73	Convergence of the density functional one-centre expansion for the molecular continuum: N 2 and (CH 3) 3 N. Theoretical Chemistry Accounts, 1999, 101, 247-256.	0.5	25
74	Evaluation of the donor ability of phenanthrolines in iridium complexes by means of synchrotron radiation photoemission spectroscopy and DFT calculations. Dalton Transactions, 2007, , 133-142.	1.6	25
75	Physico-Chemical Characteristics of Gold Nanoparticles. Comprehensive Analytical Chemistry, 2014, 66, 81-152.	0.7	25
76	Accurate local density photoionization cross sections byLCAO Stieltjes imaging approach. International Journal of Quantum Chemistry, 1995, 53, 229-244.	1.0	24
77	A new timeâ€dependent densityâ€functional method for molecular plasmonics: Formalism, implementation, and the Au₁₄₄(SH)₆₀ case study. International Journal of Quantum Chemistry, 2016, 116, 1603-1611.	1.0	24
78	Molecular Magnetic Quantum Dots in Multivalent Metal Cluster Compounds. Physical Review Letters, 1998, 81, 3211-3214.	2.9	23
79	Valence and core photoionization dynamics of acetylene by TD-DFT continuum approach. Chemical Physics, 2004, 298, 141-153.	0.9	23
80	Time dependent density functional investigation of the near-edge absorption spectra of V2O5. Physical Chemistry Chemical Physics, 2006, 8, 4300.	1.3	23
81	The role of exchange and correlation in time-dependent density-functional theory for photoionization. Journal of Chemical Physics, 2001, 114, 7816-7829.	1.2	22
82	Response function study of CO photoionization: ab initio SCF and density functional results. Chemical Physics, 2001, 272, 15-25.	0.9	22
83	Theoretical study of the photoionization shape resonances of cobaltocene and nickelocene. Chemical Physics, 2001, 273, 117-133.	0.9	21
84	Relativistic density functional study of gold coated magnetic nickel clusters. Journal of Chemical Physics, 2001, 114, 5207-5215.	1.2	21
85	Ligand-Enhanced Optical Response of Gold Nanomolecules and Its Fragment Projection Analysis: The Case of Au₃₀(SR)₁₈. Journal of Physical Chemistry C, 2017, 121, 10832-10842.	1.5	21
86	Chirality in bare and ligand-protected metal nanoclusters. Advances in Physics: X, 2018, 3, 1509727.	1.5	21
87	Photoionization of first and second row hydrides by the B-spline one-centre expansion density functional method. Journal of Electron Spectroscopy and Related Phenomena, 1998, 94, 195-209.	0.8	20
88	Spin-orbit relativistic calculations of the core excitation spectra of SO2. Journal of Chemical Physics, 2007, 126, 134308.	1.2	20
89	Photoionization of M@C60 (M=Li, Na, K) by large-scale one-centre density functional explicit continuum wave-function. Chemical Physics Letters, 1999, 309, 129-135.	1.2	19
90	Density functional calculations of valence and core photoionization of C6H6 with an exchange-correlation potential with the correct asymptotic behaviour. Physical Chemistry Chemical Physics, 2001, 3, 19-28.	1.3	19

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91	Donor Properties of Diphosphine Ligands in Tungsten Carbonyl Complexes:Â Synchrotron Radiation XPS Measurements and DFT Calculations. Organometallics, 2004, 23, 5219-5225.	1.1	19
92	Theoretical study of the Cl1s and 2p near edge photoabsorption spectra of HCl by accurate ab-initio configuration interaction and density functional approaches. Chemical Physics, 1998, 232, 9-23.	0.9	18
93	Theory of Time-Resolved Photoelectron Imaging: Nonperturbative Calculation for an Internally Converting Polyatomic Molecule. Physical Review Letters, 2002, 89, 233002.	2.9	18
94	Strong Oscillations in Molecular Valence Photoemission Intensities. Physical Review Letters, 2005, 95, 263401.	2.9	18
95	Optical Properties of Pt and Agâ€“Pt Nanoclusters from TDDFT Calculations: Plasmon Suppression by Pt Poisoning. Journal of Physical Chemistry C, 2014, 118, 28101-28108.	1.5	18
96	Electronic properties of the boroxineâ€“gold interface: evidence of ultra-fast charge delocalization. Chemical Science, 2017, 8, 3789-3798.	3.7	18
97	Intense fluorescence of Au20. Journal of Chemical Physics, 2017, 147, 074301.	1.2	18
98	Photoionization of mercury: A relativistic time-dependent density-functional-theory approach. Physical Review A, 2002, 66, .	1.0	17
99	Photoionization of oriented molecules: a time dependent density functional approach. Chemical Physics Letters, 2002, 356, 153-160.	1.2	17
100	Site-specific photoemission dynamics of N2O molecules probed by fixed-molecule core-level photoelectron angular distributions. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 29-47.	0.6	17
101	Perfluoro effects in the occupied and virtual valence orbitals of hexafluorobenzene. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 2939-2959.	0.6	17
102	Spin-orbit effects in the photoabsorption of WAu12 and MoAu12: A relativistic time dependent density functional study. Journal of Chemical Physics, 2008, 128, 134307.	1.2	17
103	N 1s photoelectron angular distributions from fixed-in-space NO2 molecules: Stereodynamics and symmetry considerations. Journal of Chemical Physics, 2010, 133, 164301.	1.2	17
104	Vibrationally resolved NEXAFS at C and N K-edges of pyridine, 2-fluoropyridine and 2,6-difluoropyridine: A combined experimental and theoretical assessment. Journal of Chemical Physics, 2015, 143, 204102.	1.2	17
105	Comment on â€œ(Auâ€“Ag)₁₄₄(SR)₆₀alloy nanomoleculesâ€•by C. Kumara and A. Dass, Nanoscale, 2011,3, 3064. Nanoscale, 2015, 7, 8166-8167.	2.8	17
106	New approach for a complete experiment: C1s photoionization in CO₂molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, F241-F250.	0.6	16
107	Theoretical study on the photoabsorption of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:mtext>M</mml:mtext><mml:msubsup><mml:mrow><mml:mtext>Au</mml:mtext></mml:mrow> (M = V, Nb and Ta). Chemical Physics Letters, 2008, 462, 358-364.	1.2	16
108	Density Functional Theory Simulation of NEXAFS Spectra of Molecules Adsorbed on Surfaces: C₂H₄ on Si(100) Case Study. Journal of Physical Chemistry C, 2012, 116, 18910-18919.	1.5	16

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109	N1s and C1s Near-Edge X-ray Absorption Fine Structure Spectra of Model Systems for Pyridine on Si(100): A DFT Simulation. Journal of Physical Chemistry C, 2014, 118, 1049-1061.	1.5	16
110	Essential dynamics for the study of microstructures in liquids. Journal of Computational Chemistry, 2015, 36, 399-407.	1.5	16
111	Theoretical study of the excited and continuum states in the NEXAFS regions of Cl2. Physical Chemistry Chemical Physics, 1999, 1, 1405-1414.	1.3	15
112	Gold-thiolate complexes: a density functional study of geometry and electronic structure. Computational and Theoretical Chemistry, 2000, 527, 63-74.	1.5	15
113	Dramatic response effects in the photoionization of the second-row hydrides:â€‚A time-dependent density functional investigation. Journal of Chemical Physics, 2003, 118, 10051-10064.	1.2	15
114	Core excitations in MgO: a DFT study with cluster models. Chemical Physics, 2005, 309, 49-58.	0.9	15
115	Extensive study on the C 1s photoionization of CS₂molecules by multi-coincidence velocity-map imaging spectrometry. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, 4033-4046.	0.6	15
116	Multiple-scattering calculations for 1s photoelectron angular distributions from single oriented molecules in the energy region above 50eV. Journal of Electron Spectroscopy and Related Phenomena, 2012, 185, 535-545.	0.8	15
117	Delocalization of a Vacancy across Two Neon Atoms Bound by the van der Waals Force. Physical Review Letters, 2016, 117, 263001.	2.9	15
118	AgPd, AuPd, and AuPt Nanoalloys with Ag- or Au-Rich Compositions: Modeling Chemical Ordering and Optical Properties. Journal of Physical Chemistry C, 2021, 125, 17372-17384.	1.5	15
119	Molecular photoionization cross sections by the local density LCAO Stieltjes imaging approach. Journal of Electron Spectroscopy and Related Phenomena, 1995, 74, 29-43.	0.8	14
120	Photoionization of zinc by TDLDA calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 4481-4487.	0.6	14
121	Fe L-Edge X-ray Absorption Spectra of Fe(II) Polypyridyl Spin Crossover Complexes from Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2013, 117, 14075-14085.	1.1	14
122	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.	1.5	14
123	TDLDA calculations of photoionization cross-section and asymmetry parameter profiles of alkaline-earth atoms. Chemical Physics, 1997, 222, 197-213.	0.9	13
124	Photoionization of CH4, SiH4, BH3 and AlH3 by the B-spline one-centre expansion density functional method. Journal of Electron Spectroscopy and Related Phenomena, 1999, 104, 135-144.	0.8	13
125	TDDFT Calculations of NEXAFS Spectra of Model Systems for SO₂ Adsorbed on the MgO (100) Surface. Journal of Physical Chemistry C, 2007, 111, 13554-13563.	1.5	13
126	Partial photoionization cross sections of C60 and C70: A gas versus adsorbed phase comparison. Surface Science, 2010, 604, 1940-1944.	0.8	13

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127	A study of the valence shell electronic states of pyridazine by photoabsorption spectroscopy and time-dependent density functional theory calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 2013, 46, 175103.	0.6	13
128	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.	2.3	13
129	Crystal Structure of Au_{36-x}Ag_x(SPh-tBu)₂₄ Nanoalloy and the Role of Ag Doping in Excited State Coupling. Journal of Physical Chemistry C, 2019, 123, 29484-29494.	1.5	13
130	Study of the electronic structure of short chain oligothiophenes. Journal of Chemical Physics, 2017, 146, 054303.	1.2	12
131	Predictions of Chemical Shifts for Reactive Intermediates in CO2 Reduction under Operando Conditions. ACS Applied Materials & Interfaces, 2021, 13, 31554-31560.	4.0	12
132	Predictive optical photoabsorption of Ag24Au(DMBT)18â^' via efficient TDDFT simulations. Journal of Chemical Physics, 2021, 155, 084103.	1.2	12
133	LCAO density functional calculations of core binding energy shifts of large molecules. Journal of Electron Spectroscopy and Related Phenomena, 1994, 69, 197-206.	0.8	11
134	Computational investigation of the L2,3-edge spectra of bulk and (110) surface of rutile TiO2. Surface Science, 2011, 605, 500-506.	0.8	11
135	Molecular-frame photoelectron angular distribution imaging studies of OCS S1s photoionization. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 194005.	0.6	11
136	Recoil frame photoelectron angular distributions of BF3: A sensitive probe of the shape resonance in the F 1s continuum. Journal of Chemical Physics, 2012, 136, 074305.	1.2	11
137	L2,3 edge photoabsorption spectra of bulk V2O5: A two components relativistic time dependent density functional theory description with finite cluster model. Journal of Chemical Physics, 2012, 137, 224308.	1.2	11
138	Optical Properties and Chemical Ordering of Agâ€“Pt Nanoalloys: A Computational Study. Journal of Physical Chemistry C, 2019, 123, 25482-25491.	1.5	11
139	Ab initio and density functional calculations of core excitation spectra of CO, H2CO and F2CO. Chemical Physics, 1996, 210, 447-459.	0.9	10
140	Photoionization cross section and angular distribution calculations of carbon tetrafluoride. Journal of Chemical Physics, 2006, 124, 214313.	1.2	10
141	2-amino-1-propanol versus 1-amino-2-propanol: Valence band and C 1s core-level photoelectron spectra. Journal of Chemical Physics, 2007, 127, 144312.	1.2	10
142	A study of the valence shell electronic structure of hexafluorobenzene using photoabsorption and photoelectron spectroscopy, and TDDFT calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 245201.	0.6	10
143	Theoretical study of sulfur L-edge XANES of thiol protected gold nanoparticles. Physical Chemistry Chemical Physics, 2011, 13, 480-487.	1.3	10
144	Photoabsorption and S 2p photoionization of the SF6 molecule: Resonances in the excitation energy range of 200â€“280 eV. Journal of Chemical Physics, 2011, 134, 174311.	1.2	10

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145	Off-resonance photoemission dynamics studied by recoil frame F1s and C1s photoelectron angular distributions of CH3F. Journal of Chemical Physics, 2014, 140, 044305.	1.2	10
146	S2p core level spectroscopy of short chain oligothiophenes. Journal of Chemical Physics, 2017, 147, 244301.	1.2	10
147	Au₃₆(SePh)₂₄ nanomolecules: synthesis, optical spectroscopy and theoretical analysis. Physical Chemistry Chemical Physics, 2018, 20, 13255-13262.	1.3	10
148	An efficient hybrid scheme for time dependent density functional theory. Journal of Chemical Physics, 2020, 152, 184104.	1.2	10
149	High resolution inner-shell spectroscopy and ab initio CI calculations on TiCl4 and isoelectronic moleculesElectronic supplementary information (ESI) available: All excitation energies and oscillator strengths for TiCl4, VOCl3, CrO2Cl2 and MnO3Cl, including Rydberg levels. See http://www.rsc.org/suppdata/cp/b3/b302805b/. Physical Chemistry Chemical Physics, 2003, 5, 2758.	1.3	9
150	A density functional theory (DFT) study on gas-phase proton transfer reactions of derivatized and underivatized peptide ions generated by matrix-assisted laser desorption ionization. Journal of the American Society for Mass Spectrometry, 2009, 20, 1327-1333.	1.2	9
151	Computational characterization of the HOMO-2 photoemission intensity oscillations in C60. Chemical Physics Letters, 2011, 516, 154-157.	1.2	9
152	Computational Study of Amino Mediated Molecular Interaction Evidenced in N 1s NEXAFS: 1,4-Diaminobenzene on Au (111). Journal of Physical Chemistry C, 2015, 119, 1988-1995.	1.5	9
153	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.	1.0	9
154	Continuum Electronic States: The Tiresia Code. Molecules, 2022, 27, 2026.	1.7	9
155	Theoretical description of the NEXAFS Cl 1s and 2p spectra of ClF and ClF3. Chemical Physics, 1999, 246, 127-145.	0.9	8
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