Mauro Stener

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/8952730/publications.pdf

Version: 2024-02-01

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	PECD study of a single-conformer molecule: a critical comparison of experiment and theory. Physical Chemistry Chemical Physics, 2022, , .	1.3	1
2	Continuum Electronic States: The Tiresia Code. Molecules, 2022, 27, 2026.	1.7	9
3	Plasmonic Circular Dichroism in Chiral Gold Nanowire Dimers. Molecules, 2022, 27, 93.	1.7	5
4	Computational NEXAFS Characterization of Molecular Model Systems for 2D Boroxine Frameworks. Nanomaterials, 2022, 12, 1610.	1.9	1
5	Revealing the electronic properties of the Bâ€“B bond: the bis-catecholato diboron molecule. Physical Chemistry Chemical Physics, 2021, 23, 23517-23525.	1.3	2
6	Theoretical Investigation of Photoinduced Processes in Subnanometer Oxide-Supported Metal Catalysts. Journal of Physical Chemistry C, 2021, 125, 2022-2032.	1.5	4
7	2p x-ray absorption spectroscopy of 3d transition metal systems. Journal of Electron Spectroscopy and Related Phenomena, 2021, 249, 147061.	0.8	44
8	Predictions of Chemical Shifts for Reactive Intermediates in CO2 Reduction under Operando Conditions. ACS Applied Materials & Interfaces, 2021, 13, 31554-31560.	4.0	12
9	Circularly Polarized Plasmons in Chiral Gold Nanowires via Quantum-Mechanical Design. Journal of Physical Chemistry Letters, 2021, 12, 5829-5835.	2.1	4
10	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
11	Predictive optical photoabsorption of Ag24Au(DMBT)18â^' via efficient TDDFT simulations. Journal of Chemical Physics, 2021, 155, 084103.	1.2	12
12	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.	2.3	8
13	Optical Activity of Metal Nanoclusters Deposited on Regular and Doped Oxide Supports from First-Principles Simulations. Molecules, 2021, 26, 6961.	1.7	2
14	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.	1.5	3
15	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
16	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
17	An efficient hybrid scheme for time dependent density functional theory. Journal of Chemical Physics, 2020, 152, 184104.	1.2	10
18	Probing gaseous molecular structure by molecular-frame photoelectron angular distributions. Journal of Chemical Physics, 2019, 151, 104302.	1.2	7

#	Article	IF	Citations
19	Optical Properties and Chemical Ordering of Agâ€“Pt Nanoalloys: A Computational Study. Journal of Physical Chemistry C, 2019, 123, 25482-25491.	1.5	11
20	Theory meets experiment for unravelling the C1s X-ray photoelectron spectra of pyridine, 2-fluoropyridine, and 2,6-difluoropyridine. Journal of Chemical Physics, 2019, 151, 124105.	1.2	6
21	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
22	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.	1.3	6
23	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
24	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
25	Theoretical study of ultrafast x-ray photoelectron diffraction from molecules undergoing photodissociation. Journal of Chemical Physics, 2018, 148, 124101.	1.2	7
26	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
27	Time-resolved photoelectron angular distributions from nonadiabatically aligned CO2 molecules with SX-FEL at SACLA. Journal of Physics Communications, 2018, 2, 115015.	0.5	7
28	Chirality in bare and ligand-protected metal nanoclusters. Advances in Physics: X, 2018, 3, 1509727.	1.5	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.	1.1	4
30	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
31	Au₃₆(SePh)₂₄ nanomolecules: synthesis, optical spectroscopy and theoretical analysis. Physical Chemistry Chemical Physics, 2018, 20, 13255-13262.	1.3	10
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.	2.3	13
33	Optical Properties of Metal Nanoclustersâ€”Theory. , 2018, , 534-545.		4
34	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
35	Study of the electronic structure of short chain oligothiophenes. Journal of Chemical Physics, 2017, 146, 054303.	1.2	12
36	Electronic properties of the boroxineâ€“gold interface: evidence of ultra-fast charge delocalization. Chemical Science, 2017, 8, 3789-3798.	3.7	18

#	Article	IF	Citations
37	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
38	Au₃₈(SPh)₂₄: Au₃₈ Protected with Aromatic Thiolate Ligands. Journal of Physical Chemistry Letters, 2017, 8, 1530-1537.	2.1	33
39	Au₂₁S(SAdm)₁₅: An Anisotropic Gold Nanomolecule. Optical and Photoluminescence Spectroscopy and First-Principles Theoretical Analysis. Journal of Physical Chemistry Letters, 2017, 8, 457-462.	2.1	8
40	Intense fluorescence of Au20. Journal of Chemical Physics, 2017, 147, 074301.	1.2	18
41	Photoelectron circular dichroism of isopropanolamine. Chemical Physics, 2017, 482, 294-302.	0.9	5
42	S2p core level spectroscopy of short chain oligothiophenes. Journal of Chemical Physics, 2017, 147, 244301.	1.2	10
43	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
44	Optical absorption of (Ag-Au)133(SCH3)52 bimetallic monolayer-protected clusters. Progress in Natural Science: Materials International, 2016, 26, 467-476.	1.8	2
45	Delocalization of a Vacancy across Two Neon Atoms Bound by the van der Waals Force. Physical Review Letters, 2016, 117, 263001.	2.9	15
46	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
47	A study of the valence shell electronic states of s-triazine by photoabsorption spectroscopy and ab initio calculations. Chemical Physics, 2016, 477, 96-104.	0.9	4
48	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
49	Chemistry of the Methylamine Termination at a Gold Surface: From Autorecognition to Condensation. Journal of Physical Chemistry C, 2016, 120, 6104-6115.	1.5	8
50	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
51	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
52	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
53	Diffraction effects in the Recoil-Frame Photoelectron Angular Distributions of Halomethanes. Journal of Physics: Conference Series, 2015, 635, 112020.	0.3	1
54	Designing ligand-enhanced optical absorption of thiolated gold nanoclusters. Chemical Communications, 2015, 51, 7935-7938.	2.2	31

#	Article	IF	Citations
55	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
56	Essential dynamics for the study of microstructures in liquids. Journal of Computational Chemistry, 2015, 36, 399-407.	1.5	16
57	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
58	Selecting core-hole localization or delocalization in CS2 by photofragmentation dynamics. Nature Communications, 2015, 6, 6166.	5.8	59
59	A study of the valence shell electronic structure and photoionisation dynamics of s-triazine. Chemical Physics, 2015, 450-451, 115-124.	0.9	1
60	Optical properties of nanoalloys. Physical Chemistry Chemical Physics, 2015, 17, 27952-27967.	1.3	45
61	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
62	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
63	Vibrationally resolved high-resolution NEXAFS and XPS spectra of phenanthrene and coronene. Journal of Chemical Physics, 2014, 141, 044313.	1.2	47
64	Imaging molecular structure through femtosecond photoelectron diffraction on aligned and oriented gas-phase molecules. Faraday Discussions, 2014, 171, 57-80.	1.6	55
65	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
66	Physico-Chemical Characteristics of Gold Nanoparticles. Comprehensive Analytical Chemistry, 2014, 66, 81-152.	0.7	25
67	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
68	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
69	Optical Properties of Silver Nanoshells from Time-Dependent Density Functional Theory Calculations. Journal of Physical Chemistry C, 2014, 118, 12450-12458.	1.5	38
70	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
71	Conformational Sensitivity in Photoelectron Circular Dichroism of 3â€Methylcyclopentanone. ChemPhysChem, 2013, 14, 1723-1732.	1.0	35
72	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

#	Article	IF	Citations
73	The near-edge X-ray-absorption fine-structure of O2 chemisorbed on Ag(110) surface studied by density functional theory. Surface Science, 2013, 616, 178-185.	0.8	4
74	Photoelectron spectroscopy and circular dichroism of a chiral metalâ€“organic complex. Rendiconti Lincei, 2013, 24, 269-275.	1.0	5
75	Gold Nanowires: A Time-Dependent Density Functional Assessment of Plasmonic Behavior. Journal of Physical Chemistry C, 2013, 117, 17196-17204.	1.5	60
76	Angular Correlation Between B K-VV Auger Electrons of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>BF</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Molecules and Coincident Fragment Ions: Manifestation of the Difference Between the Angular Correlation and Molecular Frame Auger Electron Angular Distribution. Physical Review Letters, 2013, 110, 043001.	2.9	5
77	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
78	Femtosecond photoelectron diffraction on laser-aligned molecules: Towards time-resolved imaging of molecular structure. Physical Review A, 2013, 88, .	1.0	76
79	Giant correlation effects in the photoelectron spectrum of Ni(C3H5)2: clues from accurate calculation of ionization cross-sections. Highlights in Theoretical Chemistry, 2013, , 245-253.	0.0	0
80	Recoil frame photoelectron angular distributions in core O 1s ionization of H2CO. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 194004.	0.6	4
81	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
82	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
83	Appearance of Plasmons in Fullerenes. Journal of Physics: Conference Series, 2012, 388, 022087.	0.3	2
84	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
85	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
86	Resonant Circular Dichroism of Chiral Metal-Organic Complex. Physical Review Letters, 2012, 108, 083001.	2.9	46
87	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
88	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
89	Giant correlation effects in the photoelectron spectrum of Ni(C3H5)2: clues from accurate calculation of ionization cross-sections. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	1
90	Theoretical study of sulfur L-edge XANES of thiol protected gold nanoparticles. Physical Chemistry Chemical Physics, 2011, 13, 480-487.	1.3	10

#	Article	IF	Citations
91	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
92	Optical Properties of Au Nanoclusters from TD-DFT Calculations. Journal of Physical Chemistry C, 2011, 115, 6277-6282.	1.5	100
93	The valence electronic structure and conformational flexibility of epichlorohydrin. Physical Chemistry Chemical Physics, 2011, 13, 12517.	1.3	5
94	Density Functional Study on the Morphology and Photoabsorption of CdSe Nanoclusters. Journal of Physical Chemistry C, 2011, 115, 16782-16796.	1.5	104
95	Computational characterization of the HOMO-2 photoemission intensity oscillations in C60. Chemical Physics Letters, 2011, 516, 154-157.	1.2	9
96	A study of the valence shell photoionisation dynamics of pyrimidine and pyrazine. Chemical Physics, 2011, 390, 25-35.	0.9	36
97	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
98	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
99	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
100	O1s photoionization dynamics in oriented NO2. Journal of Chemical Physics, 2011, 134, 184305.	1.2	7
101	S 2p photoabsorption of the SF5CF3 molecule: Experiment, theory and comparison with SF6. Chemical Physics, 2010, 375, 101-109.	0.9	3
102	Partial photoionization cross sections of C60 and C70: A gas versus adsorbed phase comparison. Surface Science, 2010, 604, 1940-1944.	0.8	13
103	Carbon<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>K</mml:mi></mml:mrow></mml:math>-shell photoionization of fixed-in-space<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub>	1.0	7
104	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
105	The Role of Chargeâ€“Charge Correlations and Covalent Bonding in the Electronic Structure of Adsorbed C60: C60/Al. Journal of Physical Chemistry C, 2010, 114, 18686-18692.	1.5	3
106	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
107	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
108	Conformational Effects in Photoelectron Circular Dichroism of Alaninol. ChemPhysChem, 2009, 10, 1839-1846.	1.0	45

#	Article	IF	Citations
109	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
110	Time Dependent Density Functional Theory description of giant resonances in transition metal complexes: The photoionization dynamics of Cr(CO)6. Chemical Physics, 2009, 361, 49-60.	0.9	5
111	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
112	Theoretical Study on the X-ray Absorption at the Sulfur K-Edge in Gold Nanoparticles Protected by Thiolates. Journal of Physical Chemistry C, 2009, 113, 14844-14851.	1.5	6
113	S K-edge NEXAFSspectra of model systems for SO₂on TiO₂(110): a TDDFT simulation. Physical Chemistry Chemical Physics, 2009, 11, 1146-1151.	1.3	6
114	Fluorine K-shell photoelectron angular distribution from CF4 molecules in the molecular frame. Chemical Physics Letters, 2008, 451, 182-185.	1.2	8
115	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
116	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
117	Decay Channel Dependence of the Photoelectron Angular Distributions in Core-Level Ionization of Ne Dimers. Physical Review Letters, 2008, 101, 043004.	2.9	40
118	Electrostatic effects on cluster simulation of ionic crystals and surfaces. Journal of Physics: Conference Series, 2008, 117, 012009.	0.3	0
119	Spin-orbit relativistic calculations of the core excitation spectra of SO2. Journal of Chemical Physics, 2007, 126, 134308.	1.2	20
120	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
121	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
122	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
123	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
124	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
125	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
126	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

#	Article	IF	Citations
127	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
128	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
129	Recent advances in molecular photoionization by density functional theory based approaches. Theoretical Chemistry Accounts, 2007, 117, 943-956.	0.5	34
130	Time dependent density functional investigation of the near-edge absorption spectra of V2O5. Physical Chemistry Chemical Physics, 2006, 8, 4300.	1.3	23
131	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
132	Time dependent density functional study of the photoionization dynamics of SF6. Journal of Chemical Physics, 2006, 124, 114306.	1.2	28
133	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
134	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
135	Conformational Effects on Circular Dichroism in the Photoelectron Angular Distribution. ChemPhysChem, 2006, 7, 924-934.	1.0	46
136	Photoabsorption and photoionization dynamics study of silicon tetrafluoride in the framework of time-dependent density-functional theory. Physical Review A, 2006, 73, .	1.0	6
137	Photoionization cross section and angular distribution calculations of carbon tetrafluoride. Journal of Chemical Physics, 2006, 124, 214313.	1.2	10
138	Core excitations in MgO: a DFT study with cluster models. Chemical Physics, 2005, 309, 49-58.	0.9	15
139	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
140	Angle-Resolved Photoelectron Spectroscopy of Randomly Oriented 3-Hydroxytetrahydrofuran Enantiomers. ChemPhysChem, 2005, 6, 1164-1168.	1.0	33
141	Valence photoionization dynamics in circular dichroism of chiral free molecules: The methyl-oxirane. Journal of Chemical Physics, 2005, 122, 244303.	1.2	89
142	Strong Oscillations in Molecular Valence Photoemission Intensities. Physical Review Letters, 2005, 95, 263401.	2.9	18
143	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
144	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

#	Article	IF	Citations
145	Theory of time-resolved photoelectron imaging. Comparison of a density functional with a time-dependent density functional approach. Journal of Chemical Physics, 2004, 120, 1172-1180.	1.2	5
146	Circular dichroism in photoelectron spectroscopy of free chiral molecules: Experiment and theory on methyl-oxirane. Physical Review A, 2004, 70, .	1.0	78
147	Collisional deexcitation of optically allowed excited atoms by axially symmetric molecules. Journal of Chemical Physics, 2004, 121, 9948-9958.	1.2	3
148	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
149	Valence and core photoionization dynamics of acetylene by TD-DFT continuum approach. Chemical Physics, 2004, 298, 141-153.	0.9	23
150	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
151	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
152	Origin of molecular orbital splitting of C60on Al(110). Journal of Physics Condensed Matter, 2004, 16, L407-L414.	0.7	7
153	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
154	High Resolution Inner-Shell Spectroscopy and ab initio CI Calculations on TiCl4 and Isoelectronic Molecules.. ChemInform, 2003, 34, no.	0.1	0
155	Time dependent density functional theory of core electrons excitations. Chemical Physics Letters, 2003, 373, 115-123.	1.2	232
156	Intramolecular and intermolecular Oî—¸Hî—¸O hydrogen bond in some nickel(II) complexes with tridentate aminoâ€“oxime ligands. Inorganica Chimica Acta, 2003, 355, 361-367.	1.2	4
157	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
158	3d photoionization along the xenon isoelectronic sequence. Journal of Physics B: Atomic, Molecular and Optical Physics, 2003, 36, 3097-3118.	0.6	6
159	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
160	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
161	Theory of Time-Resolved Photoelectron Imaging: Nonperturbative Calculation for an Internally Converting Polyatomic Molecule. Physical Review Letters, 2002, 89, 233002.	2.9	18
162	Photoionization of mercury: A relativistic time-dependent density-functional-theory approach. Physical Review A, 2002, 66, .	1.0	17

#	Article	IF	Citations
163	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
164	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
165	Convergence of the multicenter B-spline DFT approach for the continuum. Chemical Physics, 2002, 276, 25-43.	0.9	129
166	Time dependent density functional photoionization of CH4, NH3, H2O and HF. Chemical Physics, 2002, 282, 337-351.	0.9	48
167	Time dependent density functional study of the symmetry resolved N 1s photoionization in N2. Chemical Physics Letters, 2002, 351, 469-474.	1.2	27
168	Photoionization of oriented molecules: a time dependent density functional approach. Chemical Physics Letters, 2002, 356, 153-160.	1.2	17
169	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
170	Theoretical study of the valence and core photoemission spectra of C60. Physical Chemistry Chemical Physics, 2001, 3, 4481-4487.	1.3	36
171	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
172	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
173	Theoretical Study of Photoionization Processes in Fe(C5H5)2. Journal of Physical Chemistry A, 2001, 105, 9800-9812.	1.1	6
174	Response function study of CO photoionization: ab initio SCF and density functional results. Chemical Physics, 2001, 272, 15-25.	0.9	22
175	Theoretical study of the photoionization shape resonances of cobaltocene and nickelocene. Chemical Physics, 2001, 273, 117-133.	0.9	21
176	High energy oscillations in the valence photoionization partial cross-section of C60. Chemical Physics Letters, 2001, 348, 363-367.	1.2	30
177	Photoionization of [(Î·-C[sub 6]H[sub 6])[sub 2]Cr] with the explicit continuum B-spline density-functional method. Journal of Chemical Physics, 2001, 114, 306.	1.2	8
178	Relativistic density functional study of gold coated magnetic nickel clusters. Journal of Chemical Physics, 2001, 114, 5207-5215.	1.2	21
179	Gold-thiolate complexes: a density functional study of geometry and electronic structure. Computational and Theoretical Chemistry, 2000, 527, 63-74.	1.5	15
180	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

#	Article	IF	Citations
181	Time-dependent density functional calculations of molecular photoionization cross sections: N2 and PH3. Journal of Chemical Physics, 2000, 112, 10871-10879.	1.2	66
182	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
183	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
184	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
185	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
186	Theoretical description of the NEXAFS Cl 1s and 2p spectra of ClF and ClF3. Chemical Physics, 1999, 246, 127-145.	0.9	8
187	Relativistic density functional study on the bimetallic cluster [Pt3Fe3(CO)15]nâ" (n=0, 1, 2). Inorganica Chimica Acta, 1999, 286, 30-36.	1.2	8
188	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
189	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
190	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
191	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
192	Valence photoionization of C6H6 by the B-spline one-centre expansion density functional method. Chemical Physics, 1998, 234, 95-109.	0.9	55
193	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
194	Molecular Magnetic Quantum Dots in Multivalent Metal Cluster Compounds. Physical Review Letters, 1998, 81, 3211-3214.	2.9	23
195	Photoionization of zinc by TDLDA calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 1997, 30, 4481-4487.	0.6	14
196	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
197	TDLDA calculations of photoionization cross-section and asymmetry parameter profiles of alkaline-earth atoms. Chemical Physics, 1997, 222, 197-213.	0.9	13
198	Ab initio and density functional calculations of core excitation spectra of CO, H2CO and F2CO. Chemical Physics, 1996, 210, 447-459.	0.9	10

#	Article	IF	Citations
199	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
200	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
201	Accurate local density photoionization cross sections byLCAO Stieltjes imaging approach. International Journal of Quantum Chemistry, 1995, 53, 229-244.	1.0	24
202	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
203	Calculations of giant resonances and cross section profiles of valence ionizations of cubane by the LCAO Density Functional Stieltjes Imaging approach. Computational and Theoretical Chemistry, 1995, 357, 125-139.	1.5	3
204	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
205	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
206	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