Piero Decleva

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5900047/publications.pdf

Version: 2024-02-01

120	5,072	94381	95218
papers	citations	37 h-index	68 g-index

125	125	125	2928
all docs	docs citations	times ranked	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	Strong chiral response in non-collinear high harmonic generation driven by purely electric-dipole interactions. Optics Express, 2022, 30, 4659.	1.7	11
3	Photoelectron Circular Dichroism as a Probe of Chiral Hydrocarbons. Chemistry, 2022, 4, 31-41.	0.9	3
4	Photoionization Observables from Multi-Reference Dyson Orbitals Coupled to B-Spline DFT and TD-DFT Continuum. Molecules, 2022, 27, 1203.	1.7	11
5	Multi-electron excitation contributions towards primary and satellite states in the photoelectron spectrum. Physical Chemistry Chemical Physics, 2022, 24, 8329-8343.	1.3	7
6	Vibrationally resolved photoelectron angular distributions of ammonia. Physical Chemistry Chemical Physics, 2022, 24, 7700-7712.	1.3	1
7	Continuum Electronic States: The Tiresia Code. Molecules, 2022, 27, 2026.	1.7	9
8	Attosecond photoionisation time delays reveal the anisotropy of the molecular potential in the recoil frame. Nature Communications, 2022, 13, 1242.	5.8	28
9	Scattering effects from neighboring atoms in core-level <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mr photoemission. Physical Review B, 2022, 105, .	1.1	0
10	Discrimination of Excited States of Acetylacetone through Theoretical Molecular-Frame Photoelectron Angular Distributions. Molecules, 2022, 27, 1811.	1.7	0
11	Basic studies toward ultrafast soft x-ray photoelectron diffraction; its application to probing local structure in iodobenzene molecules. Structural Dynamics, 2022, 9, 024303.	0.9	2
12	Multireference Approach to Normal and Resonant Auger Spectra Based on the One-Center Approximation. Journal of Chemical Theory and Computation, 2022, 18, 4387-4407.	2.3	9
13	Molecular fragmentation as a way to reveal early electron dynamics induced by attosecond pulses. Faraday Discussions, 2021, 228, 349-377.	1.6	13
14	Valence-shell photoelectron circular dichroism of ruthenium(<scp>iii</scp>)-tris-(acetylacetonato) gas-phase enantiomers. Physical Chemistry Chemical Physics, 2021, 23, 24140-24153.	1.3	6
15	Enantio-sensitive unidirectional light bending. Nature Communications, 2021, 12, 3951.	5.8	28
16	Enantio-sensitive unidirectional light bending. , 2021, , .		0
17	Capturing Correlation Effects on Photoionization Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 5064-5079.	2.3	14
18	Combined Surface-Hopping, Dyson Orbital, and B-Spline Approach for the Computation of Time-Resolved Photoelectron Spectroscopy Signals: The Internal Conversion in Pyrazine. Journal of Chemical Theory and Computation, 2021, 17, 5098-5109.	2.3	11

#	Article	IF	Citations
19	Photoionization of endohedral molecules: N2@C60. Physica Scripta, 2021, 96, 124005.	1.2	1
20	Multi-reference approach to the computation of double core-hole spectra. Journal of Chemical Physics, 2021, 155, 131101.	1.2	9
21	Structuring lightâ€™s chirality to induce enantio-sensitive light bending. , 2021, , .		0
22	Photoionization of C₆₀: Effects of Correlation on Cross Sections and Angular Distributions of Valence Subshells. Journal of Physical Chemistry A, 2020, 124, 108-125.	1.1	4
23	Attosecond timing of electron emission from a molecular shape resonance. Science Advances, 2020, 6, eaba7762.	4.7	57
24	Photoionization of pyrrole from the $$B_2$$ state: a computational study on the effects of Rydbergâ€“valence mixing. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	1
25	Accurate Description of Photoionization Dynamical Parameters. Journal of Physical Chemistry Letters, 2020, 11, 5330-5337.	2.1	26
26	Structuring Lightâ€™s Chirality: LR 6= RL. , 2020, , .		0
27	Energy-Dependent Relative Cross Sections in Carbon 1s Photoionization: Separation of Direct Shake and Inelastic Scattering Effects in Single Molecules. Journal of Physical Chemistry A, 2019, 123, 7619-7636.	1.1	12
28	Ultrasensitive Chiral Spectroscopy by Dynamical Symmetry Breaking in High Harmonic Generation. Physical Review X, 2019, 9, .	2.8	55
29	Synthetic chiral light for efficient control of chiral lightâ€“matter interaction. Nature Photonics, 2019, 13, 866-871.	15.6	132
30	Probing gaseous molecular structure by molecular-frame photoelectron angular distributions. Journal of Chemical Physics, 2019, 151, 104302.	1.2	7
31	Full-dimensional theoretical description of vibrationally resolved valence-shell photoionization of H2O. Structural Dynamics, 2019, 6, 054101.	0.9	7
32	Electron correlation effects in the photoionization of CO and isoelectronic diatomic molecules. Physical Chemistry Chemical Physics, 2019, 21, 1937-1951.	1.3	8
33	Multi-slit-type interference in carbon 2s photoionization of polyatomic molecules: from a fundamental effect to structural parameters. Physical Chemistry Chemical Physics, 2019, 21, 13600-13610.	1.3	0
34	Resonant Photoelectron Confinement in the SF₆ Molecule. Journal of Physical Chemistry A, 2019, 123, 1062-1068.	1.1	5
35	Ultrafast All-Optical Detection of Chiral Degrees of Freedom by Symmetry Breaking High Harmonic Spectroscopy. , 2019, , .		0
36	Chiral dichroism in bi-elliptical high-order harmonic generation. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 06LT01.	0.6	25

#	Article	IF	Citations
37	Acetylacetone photodynamics at a seeded free-electron laser. Nature Communications, 2018, 9, 63.	5.8	72
38	Theoretical study of ultrafast x-ray photoelectron diffraction from molecules undergoing photodissociation. Journal of Chemical Physics, 2018, 148, 124101.	1.2	7
39	Multi-channel dynamics in high harmonic generation of aligned CO₂: ab initio analysis with time-dependent B-spline algebraic diagrammatic construction. Physical Chemistry Chemical Physics, 2018, 20, 8311-8325.	1.3	54
40	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
41	Strong-field control and enhancement of chiral response in bi-elliptical high-order harmonic generation: an analytical model. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 124002.	0.6	22
42	Attosecond Pumpâ€“Probe Spectroscopy of Charge Dynamics in Tryptophan. Journal of Physical Chemistry Letters, 2018, 9, 4570-4577.	2.1	74
43	Realâ€Time Imaging of Ultrafast Charge Dynamics in Tetrafluoromethane from Attosecond Pumpâ€Probe Photoelectron Spectroscopy. Chemistry - A European Journal, 2018, 24, 12061-12070.	1.7	16
44	Role of electron-nuclear coupled dynamics on charge migration induced by attosecond pulses in glycine. Chemical Physics Letters, 2017, 683, 357-364.	1.2	34
45	Attosecond Electron Dynamics in Molecules. Chemical Reviews, 2017, 117, 10760-10825.	23.0	367
46	Ultrafast charge dynamics in glycine induced by attosecond pulses. Physical Chemistry Chemical Physics, 2017, 19, 19767-19776.	1.3	34
47	Photoelectron recoil in CO in the x-ray region up to 7 keV. Physical Review A, 2017, 95, .	1.0	12
48	Photoelectron circular dichroism of isopropanolamine. Chemical Physics, 2017, 482, 294-302.	0.9	5
49	Interference effects in photoelectron asymmetry parameter (Î²) trends of C 2sâ^'1states of ethyne, ethene and ethane. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 235102.	0.6	2
50	Photoionization of furan from the ground and excited electronic states. Journal of Chemical Physics, 2016, 144, 084307.	1.2	20
51	A Multichannel Least-Squares B-Spline Approach to Molecular Photoionization: Theory, Implementation, and Applications within the Configurationâ€“Interaction Singles Approximation. Journal of Chemical Theory and Computation, 2016, 12, 4996-5008.	2.3	34
52	Decoherence, control and attosecond probing of XUV-induced charge migration in biomolecules. A theoretical outlook. Faraday Discussions, 2016, 194, 41-59.	1.6	43
53	Attosecond electronic and nuclear quantum photodynamics of ozone monitored with time and angle resolved photoelectron spectra. Scientific Reports, 2016, 6, 36613.	1.6	4
54	Photoelectron diffraction in methane probed via vibrationally resolved inner-valence photoionization cross-section ratios. Physical Chemistry Chemical Physics, 2016, 18, 3214-3222.	1.3	4

#	Article	IF	Citations
55	Selecting core-hole localization or delocalization in CS2 by photofragmentation dynamics. Nature Communications, 2015, 6, 6166.	5.8	59
56	Timescales of Nâ€“H bond dissociation in pyrrole: a nonadiabatic dynamics study. Physical Chemistry Chemical Physics, 2015, 17, 19012-19020.	1.3	40
57	Vibrationally Resolved B 1s Photoionization Cross Section of BF₃. Journal of Physical Chemistry A, 2015, 119, 5971-5978.	1.1	12
58	Ultrafast Charge Dynamics in an Amino Acid Induced by Attosecond Pulses. IEEE Journal of Selected Topics in Quantum Electronics, 2015, 21, 1-12.	1.9	19
59	B-spline algebraic diagrammatic construction: Application to photoionization cross-sections and high-order harmonic generation. Journal of Chemical Physics, 2014, 141, 164126.	1.2	40
60	Vibrationally resolved C 1s photoionization cross section of CF₄. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 124032.	0.6	11
61	Dynamical photoionization observables of the CS molecule: The role of electron correlation. Journal of Chemical Physics, 2014, 140, 204304.	1.2	32
62	Imaging molecular structure through femtosecond photoelectron diffraction on aligned and oriented gas-phase molecules. Faraday Discussions, 2014, 171, 57-80.	1.6	55
63	Angular Momentum Sensitive Two-Center Interference. Physical Review Letters, 2014, 112, 023001.	2.9	28
64	Ultrafast electron dynamics in phenylalanine initiated by attosecond pulses. Science, 2014, 346, 336-339.	6.0	615
65	Photoelectron Interference in Metallocenes: A Probe of Geometrical and Electronic Structure. Journal of Physical Chemistry A, 2014, 118, 6692-6698.	1.1	1
66	Dissociative and non-dissociative photoionization of molecular fluorine from inner and valence shells. Journal of Electron Spectroscopy and Related Phenomena, 2014, 195, 320-326.	0.8	6
67	Interference and diffraction in photoelectron spectra. Journal of Electron Spectroscopy and Related Phenomena, 2014, 195, 307-312.	0.8	3
68	A coupled-cluster study of photodetachment cross sections of closed-shell anions. Journal of Chemical Physics, 2014, 141, 174315.	1.2	13
69	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
70	Conformational Sensitivity in Photoelectron Circular Dichroism of 3â€Methylcyclopentanone. ChemPhysChem, 2013, 14, 1723-1732.	1.0	35
71	Photoelectron spectroscopy and circular dichroism of a chiral metalâ€“organic complex. Rendiconti Lincei, 2013, 24, 269-275.	1.0	5
72	Photoionization cross section by Stieltjes imaging applied to coupled cluster Lanczos pseudo-spectra. Journal of Chemical Physics, 2013, 139, 094103.	1.2	33

#	Article	IF	Citations
73	Laboratory-frame electron angular distributions: Probing the chemical environment through intramolecular electron scattering. Physical Review A, 2013, 87, .	1.0	14
74	Water molecules in ultrashort intense laser fields. Chemical Physics, 2013, 414, 45-52.	0.9	36
75	Intensity oscillations in the carbon 1s ionization cross sections of 2-butyne. Journal of Chemical Physics, 2013, 138, 234310.	1.2	12
76	Intramolecular photoelectron diffraction in the gas phase. Journal of Chemical Physics, 2013, 139, 124306.	1.2	39
77	From double-slit interference to structural information in simple hydrocarbons. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 15201-15206.	3.3	57
78	Femtosecond photoelectron diffraction on laser-aligned molecules: Towards time-resolved imaging of molecular structure. Physical Review A, 2013, 88, .	1.0	76
79	Relationship between polarization-averaged molecular-frame photoelectron angular distributions and geometry. Physical Review A, 2013, 88, .	1.0	22
80	Effects of molecular potential and geometry on atomic core-level photoemission over an extended energy range: The case study of the CO molecule. Physical Review A, 2013, 88, .	1.0	36
81	Vibrationally resolved photoelectron angular distributions from randomly oriented and fixed-in-space N₂and CO molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 194008.	0.6	15
82	Double-slit experiment with a polyatomic molecule: vibrationally resolved C 1s photoelectron spectra of acetylene. New Journal of Physics, 2012, 14, 033012.	1.2	40
83	Intramolecular electron diffraction in vibrationally resolved<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>K</mml:mi></mml:math>-shell photoionization of methane. Physical Review A, 2012, 85, .	1.0	37
84	Resonant Circular Dichroism of Chiral Metal-Organic Complex. Physical Review Letters, 2012, 108, 083001.	2.9	46
85	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
86	Vibrational branching ratios in the photoelectron spectra of N2 and CO: interference and diffraction effects. Physical Chemistry Chemical Physics, 2012, 14, 10853.	1.3	27
87	Density functional theory for molecular multiphoton ionization in the perturbative regime. Journal of Chemical Physics, 2012, 137, 134103.	1.2	11
88	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
89	Direct observation of Youngâ€™s double-slit interferences in vibrationally resolved photoionization of diatomic molecules. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 7793-7796.	3.3	108
90	Alignment-Dependent Ionization of<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>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CO</mml:mi>	2.9	152

#	Article	IF	Citations
91	Strong oscillations in the nondipole corrections to the photoelectron angular distributions fromC60. Physical Review A, 2010, 81, .	1.0	14
92	Conformational Effects in Photoelectron Circular Dichroism of Alaninol. ChemPhysChem, 2009, 10, 1839-1846.	1.0	45
93	Nondipolar effects in the photoionization dynamics of carbon tetrafluoride. Physical Review A, 2008, 78, .	1.0	2
94	Recent advances in molecular photoionization by density functional theory based approaches. Theoretical Chemistry Accounts, 2007, 117, 943-956.	0.5	34
95	Time dependent density functional study of the photoionization dynamics of SF6. Journal of Chemical Physics, 2006, 124, 114306.	1.2	28
96	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
97	Conformational Effects on Circular Dichroism in the Photoelectron Angular Distribution. ChemPhysChem, 2006, 7, 924-934.	1.0	46
98	Photoionization cross-sections: a guide to electronic structure. Coordination Chemistry Reviews, 2005, 249, 209-228.	9.5	54
99	Valence photoionization dynamics in circular dichroism of chiral free molecules: The methyl-oxirane. Journal of Chemical Physics, 2005, 122, 244303.	1.2	89
100	Strong Oscillations in Molecular Valence Photoemission Intensities. Physical Review Letters, 2005, 95, 263401.	2.9	18
101	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
102	Circular dichroism in photoelectron spectroscopy of free chiral molecules: Experiment and theory on methyl-oxirane. Physical Review A, 2004, 70, .	1.0	78
103	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
104	Convergence of the multicenter B-spline DFT approach for the continuum. Chemical Physics, 2002, 276, 25-43.	0.9	129
105	Time dependent density functional photoionization of CH4, NH3, H2O and HF. Chemical Physics, 2002, 282, 337-351.	0.9	48
106	Time dependent density functional study of the symmetry resolved N 1s photoionization in N2. Chemical Physics Letters, 2002, 351, 469-474.	1.2	27
107	Applications ofB-splines in atomic and molecular physics. Reports on Progress in Physics, 2001, 64, 1815-1943.	8.1	608
108	Theoretical study of the valence and core photoemission spectra of C60. Physical Chemistry Chemical Physics, 2001, 3, 4481-4487.	1.3	36

#	Article	IF	Citations
109	Response function study of CO photoionization: ab initio SCF and density functional results. Chemical Physics, 2001, 272, 15-25.	0.9	22
110	High energy oscillations in the valence photoionization partial cross-section of C60. Chemical Physics Letters, 2001, 348, 363-367.	1.2	30
111	Time-dependent density functional calculations of molecular photoionization cross sections: N2 and PH3. Journal of Chemical Physics, 2000, 112, 10871-10879.	1.2	66
112	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
113	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
114	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
115	Valence photoionization of C6H6 by the B-spline one-centre expansion density functional method. Chemical Physics, 1998, 234, 95-109.	0.9	55
116	Multichannel continuum states by a least-squares approach in a spline basis: application to He and H-photoionization. Journal of Physics B: Atomic, Molecular and Optical Physics, 1994, 27, 4867-4889.	0.6	34
117	LCAO expansion in a spline basis for accurate variational determination of continuum wavefunctions. Applications to H+2 and HeH2+. Chemical Physics, 1994, 181, 85-95.	0.9	19
118	Accurate variational determination of continuum wavefunctions by a one-centre expansion in a spline basis. An application to H+2and HeH2+photoionization. Journal of Physics B: Atomic, Molecular and Optical Physics, 1992, 25, 3345-3356.	0.6	34
119	Variational approach to continuum orbitals in a spline basis: An application to H2+ photoionization. Chemical Physics, 1992, 159, 185-196.	0.9	83
120	Continuum wavefunctions calculations with least-squares schemes in a B-splines basis. Computer Physics Communications, 1992, 71, 207-214.	3.0	33