# Piero Decleva

List of Publications by Year
in descending order

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| 120 | 5,072 | 94433 37 | 95266 68 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 125 | 125 | 125 | 2928 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Ultrafast electron dynamics in phenylalanine initiated by attosecond pulses. Science, 2014, 346, 336-339. | 12.6 | 615 |
| 2 | Applications ofB-splines in atomic and molecular physics. Reports on Progress in Physics, 2001, 64, 1815-1943. | 20.1 | 608 |
| 3 | Attosecond Electron Dynamics in Molecules. Chemical Reviews, 2017, 117, 10760-10825. | 47.7 | 367 |
| 4 | 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> | 7.8 | 152 |
| 5 | Synthetic chiral light for efficient control of chiral lightâ€“matter interaction. Nature Photonics, 2019, 13, 866-871. | 31.4 | 132 |
| 6 | Convergence of the multicenter B-spline DFT approach for the continuum. Chemical Physics, 2002, 276, 25-43. | 1.9 | 129 |
| 7 | 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, 7302-7306. | 7.1 | 108 |
| 8 | 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. | 3.0 | 91 |
| 9 | Valence photoionization dynamics in circular dichroism of chiral free molecules: The methyl-oxirane. Journal of Chemical Physics, 2005, 122, 244303. | 3.0 | 89 |
| 10 | Variational approach to continuum orbitals in a spline basis: An application to H2+ photoionization. Chemical Physics, 1992, 159, 185-196. | 1.9 | 83 |
| 11 | Circular dichroism in photoelectron spectroscopy of free chiral molecules: Experiment and theory on methyl-oxirane. Physical Review A, 2004, 70, . | 2.5 | 78 |
| 12 | Femtosecond photoelectron diffraction on laser-aligned molecules: Towards time-resolved imaging of molecular structure. Physical Review A, 2013, 88, . | 2.5 | 76 |
| 13 | Density functional study on the circular dichroism of photoelectron angular distribution from chiral derivatives of oxirane. Journal of Chemical Physics, 2004, 120, 3284-3296. | 3.0 | 74 |
| 14 | Attosecond Pumpâ€“Probe Spectroscopy of Charge Dynamics in Tryptophan. Journal of Physical Chemistry Letters, 2018, 9, 4570-4577. | 4.6 | 74 |
| 15 | Acetylacetone photodynamics at a seeded free-electron laser. Nature Communications, 2018, 9, 63. | 12.8 | 72 |
| 16 | Time-dependent density functional calculations of molecular photoionization cross sections: N2 and PH3. Journal of Chemical Physics, 2000, 112, 10871-10879. | 3.0 | 66 |
| 17 | Selecting core-hole localization or delocalization in CS2 by photofragmentation dynamics. Nature Communications, 2015, 6, 6166. | 12.8 | 59 |
| 18 | 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. | 7.1 | 57 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Attosecond timing of electron emission from a molecular shape resonance. Science Advances, 2020, 6, eaba7762. | 10.3 | 57 |
| 20 | Valence photoionization of C6H6 by the B-spline one-centre expansion density functional method. Chemical Physics, 1998, 234, 95-109. | 1.9 | 55 |
| 21 | Imaging molecular structure through femtosecond photoelectron diffraction on aligned and oriented gas-phase molecules. Faraday Discussions, 2014, 171, 57-80. | 3.2 | 55 |
| 22 | Ultrasensitive Chiral Spectroscopy by Dynamical Symmetry Breaking in High Harmonic Generation. Physical Review X, 2019, 9, . | 8.9 | 55 |
| 23 | Photoionization cross-sections: a guide to electronic structure. Coordination Chemistry Reviews, 2005, 249, 209-228. | 18.8 | 54 |
| 24 | Multi-channel dynamics in high harmonic generation of aligned CO<sub>2</sub>: ab initio analysis with time-dependent B-spline algebraic diagrammatic construction. Physical Chemistry Chemical Physics, 2018, 20, 8311-8325. | 2.8 | 54 |
| 25 | 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. | 1.5 | 53 |
| 26 | Time dependent density functional photoionization of CH4, NH3, H2O and HF. Chemical Physics, 2002, 282, 337-351. | 1.9 | 48 |
| 27 | Conformational Effects on Circular Dichroism in the Photoelectron Angular Distribution. ChemPhysChem, 2006, 7, 924-934. | 2.1 | 46 |
| 28 | Resonant Circular Dichroism of Chiral Metal-Organic Complex. Physical Review Letters, 2012, 108, 083001. | 7.8 | 46 |
| 29 | Femtosecond x-ray photoelectron diffraction on gas-phase dibromobenzene molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 124035. | 1.5 | 46 |
| 30 | Conformational Effects in Photoelectron Circular Dichroism of Alaninol. ChemPhysChem, 2009, 10, 1839-1846. | 2.1 | 45 |
| 31 | Photoionization of C60 by large scale one-center density functional explicit continuum wave-function. Journal of Chemical Physics, 1999, 111, 4589-4597. | 3.0 | 44 |
| 32 | Decoherence, control and attosecond probing of XUV-induced charge migration in biomolecules. A theoretical outlook. Faraday Discussions, 2016, 194, 41-59. | 3.2 | 43 |
| 33 | Theoretical study on the circular dichroism in core and valence photoelectron angular distributions of camphor enantiomers. Journal of Chemical Physics, 2006, 124, 024326. | 3.0 | 41 |
| 34 | Double-slit experiment with a polyatomic molecule: vibrationally resolved C 1s photoelectron spectra of acetylene. New Journal of Physics, 2012, 14, 033012. | 2.9 | 40 |
| 35 | B-spline algebraic diagrammatic construction: Application to photoionization cross-sections and high-order harmonic generation. Journal of Chemical Physics, 2014, 141, 164126. | 3.0 | 40 |
| 36 | Timescales of Nâ€“H bond dissociation in pyrrole: a nonadiabatic dynamics study. Physical Chemistry Chemical Physics, 2015, 17, 19012-19020. | 2.8 | 40 |

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| 37 | Intramolecular photoelectron diffraction in the gas phase. Journal of Chemical Physics, 2013, 139, 124306. | 3.0 | 39 |
| 38 | 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, . | 2.5 | 37 |
| 39 | Theoretical study of the valence and core photoemission spectra of C60. Physical Chemistry Chemical Physics, 2001, 3, 4481-4487. | 2.8 | 36 |
| 40 | Water molecules in ultrashort intense laser fields. Chemical Physics, 2013, 414, 45-52. | 1.9 | 36 |
| 41 | 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, . | 2.5 | 36 |
| 42 | Conformational Sensitivity in Photoelectron Circular Dichroism of 3â€Methylcyclopentanone. ChemPhysChem, 2013, 14, 1723-1732. | 2.1 | 35 |
| 43 | 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. | 1.5 | 34 |
| 44 | 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. | 1.5 | 34 |
| 45 | Recent advances in molecular photoionization by density functional theory based approaches. Theoretical Chemistry Accounts, 2007, 117, 943-956. | 1.4 | 34 |
| 46 | 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. | 5.3 | 34 |
| 47 | Role of electron-nuclear coupled dynamics on charge migration induced by attosecond pulses in glycine. Chemical Physics Letters, 2017, 683, 357-364. | 2.6 | 34 |
| 48 | Ultrafast charge dynamics in glycine induced by attosecond pulses. Physical Chemistry Chemical Physics, 2017, 19, 19767-19776. | 2.8 | 34 |
| 49 | Continuum wavefunctions calculations with least-squares schemes in a B-splines basis. Computer Physics Communications, 1992, 71, 207-214. | 7.5 | 33 |
| 50 | Photoionization cross section by Stieltjes imaging applied to coupled cluster Lanczos pseudo-spectra. Journal of Chemical Physics, 2013, 139, 094103. | 3.0 | 33 |
| 51 | Dynamical photoionization observables of the CS molecule: The role of electron correlation. Journal of Chemical Physics, 2014, 140, 204304. | 3.0 | 32 |
| 52 | High energy oscillations in the valence photoionization partial cross-section of C60. Chemical Physics Letters, 2001, 348, 363-367. | 2.6 | 30 |
| 53 | Time dependent density functional study of the photoionization dynamics of SF6. Journal of Chemical Physics, 2006, 124, 114306. | 3.0 | 28 |
| 54 | Angular Momentum Sensitive Two-Center Interference. Physical Review Letters, 2014, 112, 023001. | 7.8 | 28 |

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| 55 | Enantio-sensitive unidirectional light bending. Nature Communications, 2021, 12, 3951. | 12.8 | 28 |
| 56 | Attosecond photoionisation time delays reveal the anisotropy of the molecular potential in the recoil frame. Nature Communications, 2022, 13, 1242. | 12.8 | 28 |
| 57 | Time dependent density functional study of the symmetry resolved N 1s photoionization in N2. Chemical Physics Letters, 2002, 351, 469-474. | 2.6 | 27 |
| 58 | Vibrational branching ratios in the photoelectron spectra of N2 and CO: interference and diffraction effects. Physical Chemistry Chemical Physics, 2012, 14, 10853. | 2.8 | 27 |
| 59 | Accurate Description of Photoionization Dynamical Parameters. Journal of Physical Chemistry Letters, 2020, 11, 5330-5337. | 4.6 | 26 |
| 60 | 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. | 1.4 | 25 |
| 61 | Chiral dichroism in bi-elliptical high-order harmonic generation. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 06LT01. | 1.5 | 25 |
| 62 | Response function study of CO photoionization: ab initio SCF and density functional results. Chemical Physics, 2001, 272, 15-25. | 1.9 | 22 |
| 63 | Relationship between polarization-averaged molecular-frame photoelectron angular distributions and geometry. Physical Review A, 2013, 88, . | 2.5 | 22 |
| 64 | 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. | 1.5 | 22 |
| 65 | Photoionization of furan from the ground and excited electronic states. Journal of Chemical Physics, 2016, 144, 084307. | 3.0 | 20 |
| 66 | 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. | 1.9 | 19 |
| 67 | Ultrafast Charge Dynamics in an Amino Acid Induced by Attosecond Pulses. IEEE Journal of Selected Topics in Quantum Electronics, 2015, 21, 1-12. | 2.9 | 19 |
| 68 | Strong Oscillations in Molecular Valence Photoemission Intensities. Physical Review Letters, 2005, 95, 263401. | 7.8 | 18 |
| 69 | Realâ€Time Imaging of Ultrafast Charge Dynamics in Tetrafluoromethane from Attosecond Pumpâ€Probe Photoelectron Spectroscopy. Chemistry - A European Journal, 2018, 24, 12061-12070. | 3.3 | 16 |
| 70 | Vibrationally resolved photoelectron angular distributions from randomly oriented and fixed-in-space N<sub>2</sub>and CO molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 194008. | 1.5 | 15 |
| 71 | 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. | 1.7 | 15 |
| 72 | Strong oscillations in the nondipole corrections to the photoelectron angular distributions fromC60. Physical Review A, 2010, 81, . | 2.5 | 14 |

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| 73 | Laboratory-frame electron angular distributions: Probing the chemical environment through intramolecular electron scattering. Physical Review A, 2013, 87, . | 2.5 | 14 |
| 74 | Capturing Correlation Effects on Photoionization Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 5064-5079. | 5.3 | 14 |
| 75 | A coupled-cluster study of photodetachment cross sections of closed-shell anions. Journal of Chemical Physics, 2014, 141, 174315. | 3.0 | 13 |
| 76 | Molecular fragmentation as a way to reveal early electron dynamics induced by attosecond pulses. Faraday Discussions, 2021, 228, 349-377. | 3.2 | 13 |
| 77 | Intensity oscillations in the carbon 1s ionization cross sections of 2-butyne. Journal of Chemical Physics, 2013, 138, 234310. | 3.0 | 12 |
| 78 | Vibrationally Resolved B 1s Photoionization Cross Section of BF<sub>3</sub>. Journal of Physical Chemistry A, 2015, 119, 5971-5978. | 2.5 | 12 |
| 79 | Photoelectron recoil in CO in the x-ray region up to 7 keV. Physical Review A, 2017, 95, . | 2.5 | 12 |
| 80 | 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. | 2.5 | 12 |
| 81 | Density functional theory for molecular multiphoton ionization in the perturbative regime. Journal of Chemical Physics, 2012, 137, 134103. | 3.0 | 11 |
| 82 | Vibrationally resolved C 1s photoionization cross section of CF<sub>4</sub>. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 124032. | 1.5 | 11 |
| 83 | 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. | 5.3 | 11 |
| 84 | Strong chiral response in non-collinear high harmonic generation driven by purely electric-dipole interactions. Optics Express, 2022, 30, 4659. | 3.4 | 11 |
| 85 | Photoionization Observables from Multi-Reference Dyson Orbitals Coupled to B-Spline DFT and TD-DFT Continuum. Molecules, 2022, 27, 1203. | 3.8 | 11 |
| 86 | Multi-reference approach to the computation of double core-hole spectra. Journal of Chemical Physics, 2021, 155, 131101. | 3.0 | 9 |
| 87 | Continuum Electronic States: The Tiresia Code. Molecules, 2022, 27, 2026. | 3.8 | 9 |
| 88 | Multireference Approach to Normal and Resonant Auger Spectra Based on the One-Center Approximation. Journal of Chemical Theory and Computation, 2022, 18, 4387-4407. | 5.3 | 9 |
| 89 | Electron correlation effects in the photoionization of CO and isoelectronic diatomic molecules. Physical Chemistry Chemical Physics, 2019, 21, 1937-1951. | 2.8 | 8 |
| 90 | Theoretical study of ultrafast x-ray photoelectron diffraction from molecules undergoing photodissociation. Journal of Chemical Physics, 2018, 148, 124101. | 3.0 | 7 |

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| 91 | Time-resolved photoelectron angular distributions from nonadiabatically aligned CO2 molecules with SX-FEL at SACLA. Journal of Physics Communications, 2018, 2, 115015. | 1.2 | 7 |
| 92 | Probing gaseous molecular structure by molecular-frame photoelectron angular distributions. Journal of Chemical Physics, 2019, 151, 104302. | 3.0 | 7 |
| 93 | Full-dimensional theoretical description of vibrationally resolved valence-shell photoionization of H2O. Structural Dynamics, 2019, 6, 054101. | 2.3 | 7 |
| 94 | Multi-electron excitation contributions towards primary and satellite states in the photoelectron spectrum. Physical Chemistry Chemical Physics, 2022, 24, 8329-8343. | 2.8 | 7 |
| 95 | Dissociative and non-dissociative photoionization of molecular fluorine from inner and valence shells. Journal of Electron Spectroscopy and Related Phenomena, 2014, 195, 320-326. | 1.7 | 6 |
| 96 | Valence-shell photoelectron circular dichroism of ruthenium(<scp>iii</scp>)-tris-(acetylacetonato) gas-phase enantiomers. Physical Chemistry Chemical Physics, 2021, 23, 24140-24153. | 2.8 | 6 |
| 97 | Photoelectron spectroscopy and circular dichroism of a chiral metalâ€“organic complex. Rendiconti Lincei, 2013, 24, 269-275. | 2.2 | 5 |
| 98 | Photoelectron circular dichroism of isopropanolamine. Chemical Physics, 2017, 482, 294-302. | 1.9 | 5 |
| 99 | Resonant Photoelectron Confinement in the SF<sub>6</sub> Molecule. Journal of Physical Chemistry A, 2019, 123, 1062-1068. | 2.5 | 5 |
| 100 | Attosecond electronic and nuclear quantum photodynamics of ozone monitored with time and angle resolved photoelectron spectra. Scientific Reports, 2016, 6, 36613. | 3.3 | 4 |
| 101 | Photoelectron diffraction in methane probed via vibrationally resolved inner-valence photoionization cross-section ratios. Physical Chemistry Chemical Physics, 2016, 18, 3214-3222. | 2.8 | 4 |
| 102 | Photoionization of C<sub>60</sub>: Effects of Correlation on Cross Sections and Angular Distributions of Valence Subshells. Journal of Physical Chemistry A, 2020, 124, 108-125. | 2.5 | 4 |
| 103 | Interference and diffraction in photoelectron spectra. Journal of Electron Spectroscopy and Related Phenomena, 2014, 195, 307-312. | 1.7 | 3 |
| 104 | Photoelectron Circular Dichroism as a Probe of Chiral Hydrocarbons. Chemistry, 2022, 4, 31-41. | 2.2 | 3 |
| 105 | Nondipolar effects in the photoionization dynamics of carbon tetrafluoride. Physical Review A, 2008, 78, . | 2.5 | 2 |
| 106 | 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. | 1.5 | 2 |
| 107 | Basic studies toward ultrafast soft x-ray photoelectron diffraction; its application to probing local structure in iodobenzene molecules. Structural Dynamics, 2022, 9, 024303. | 2.3 | 2 |
| 108 | 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. | 1.4 | 1 |

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| 109 | Photoelectron Interference in Metallocenes: A Probe of Geometrical and Electronic Structure. Journal of Physical Chemistry A, 2014, 118, 6692-6698. | 2.5 | 1 |
| 110 | Photoionization of pyrrole from the $$B_2$$ state: a computational study on the effects of Rydbergâ€“valence mixing. Theoretical Chemistry Accounts, 2020, 139, 1. | 1.4 | 1 |
| 111 | Photoionization of endohedral molecules: N2@C60. Physica Scripta, 2021, 96, 124005. | 2.5 | 1 |
| 112 | PECD study of a single-conformer molecule: a critical comparison of experiment and theory. Physical Chemistry Chemical Physics, 2022, , . | 2.8 | 1 |
| 113 | Vibrationally resolved photoelectron angular distributions of ammonia. Physical Chemistry Chemical Physics, 2022, 24, 7700-7712. | 2.8 | 1 |
| 114 | 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. | 2.8 | 0 |
| 115 | Enantio-sensitive unidirectional light bending. , 2021, , . | | 0 |
| 116 | Ultrafast All-Optical Detection of Chiral Degrees of Freedom by Symmetry Breaking High Harmonic Spectroscopy. , 2019, , . | | 0 |
| 117 | Structuring Lightâ€™s Chirality: LR 6= RL. , 2020, , . | | 0 |
| 118 | Structuring lightâ€™s chirality to induce enantio-sensitive light bending. , 2021, , . | | 0 |
| 119 | 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, . | 3.2 | 0 |
| 120 | Discrimination of Excited States of Acetylacetone through Theoretical Molecular-Frame Photoelectron Angular Distributions. Molecules, 2022, 27, 1811. | 3.8 | 0 |