Andrea Peluso

List of Publications by Year
in descending order

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116 papers	2,409 citations	201575 27 h-index	289141 40 g-index
123 all docs	123 docs citations	123 times ranked	1754 citing authors

#	Article	IF	Citations
1	Dynamics of radiationless transitions in large molecular systems: A Franckâ€“Condon-based method accounting for displacements and rotations of all the normal coordinates. Journal of Chemical Physics, 2003, 119, 8437-8448.	1.2	123
2	The vibrational progressions of the Nâ†'V electronic transition of ethylene: A test case for the computation of Franck-Condon factors of highly flexible photoexcited molecules. Journal of Chemical Physics, 2006, 125, 194308.	1.2	90
3	Generating Function Approach to the Calculation of Spectral Band Shapes of Free-Base Chlorin Including Duschinsky and Herzbergâ€“Teller Effects. Journal of Physical Chemistry A, 2012, 116, 9934-9940.	1.1	78
4	Vibronic coupling in electronic transitions with significant Duschinsky effect. International Journal of Quantum Chemistry, 1997, 63, 233-244.	1.0	71
5	A Novel .eta.7 Coordination Mode of a Benzyl Ligand in a Cationic Zirconium Complex. Organometallics, 1994, 13, 3773-3775.	1.1	61
6	The temperature dependence of radiationless transition rates from ab initio computations. Physical Chemistry Chemical Physics, 2011, 13, 4420.	1.3	57
7	Direct Experimental Observation of the Effect of the Base Pairing on the Oxidation Potential of Guanine. Journal of the American Chemical Society, 2005, 127, 15040-15041.	6.6	55
8	Franckâ€“Condon factorsâ€”Computational approaches and recent developments. Canadian Journal of Chemistry, 2013, 91, 495-504.	0.6	52
9	Fluorescent salen-type Zn(II) Complexes As Probes for Detecting Hydrogen Sulfide and Its Anion: Bioimaging Applications. Inorganic Chemistry, 2020, 59, 15977-15986.	1.9	49
10	Tuning Second-Order Optical Nonlinearities in Push-Pull Benzimidazoles. European Journal of Organic Chemistry, 2004, 2004, 2620-2626.	1.2	48
11	The electron photodetachment spectrum of c-C4F8â^': A test case for the computation of Franck-Condon factors of highly flexible molecules. Journal of Chemical Physics, 2008, 128, 044303.	1.2	46
12	A series of compounds forming polar crystals and showing single-crystal-to-single-crystal transitions between polar phases. CrystEngComm, 2012, 14, 2645.	1.3	45
13	Polymerization Mechanism of Conjugated Dienes in the Presence of Zieglerâ^'Natta Type Catalysts:Â Theoretical Study of Butadiene and Isoprene Polymerization with CpTiCl3â^'MAO Initiator. Organometallics, 2000, 19, 411-419.	1.1	41
14	Franckâ€“Condon factors in curvilinear coordinates: the photoelectron spectrum of ammonia. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	38
15	Mechanism of Isoprene and Butadiene Polymerization in the Presence of CpTiCl3â^'MAO Initiator:Â A Theoretical Study. Macromolecules, 1997, 30, 2219-2227.	2.2	37
16	Photoelectron Spectrum of Ammonia, a Test Case for the Calculation of Franckâ^'Condon Factors in Molecules Undergoing Large Geometrical Displacements upon Photoionization. Journal of Physical Chemistry A, 2009, 113, 14831-14837.	1.1	36
17	Quantum Dynamics of Electron Transfer from Bacteriochlorophyll to Pheophytin in Bacterial Reaction Centers. Journal of Chemical Theory and Computation, 2007, 3, 673-680.	2.3	35
18	The Oxidation Potential of Adenosine and Adenosine-Thymidine Base Pair in Chloroform Solution. Journal of the American Chemical Society, 2007, 129, 15347-15353.	6.6	34

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19	On the Mechanism of Asymmetric Epoxidation of Enones Catalyzed by Î±,Î±â€‹scp›L‹/scp›â€Diarylprolinols: A Theoretical Insight. Advanced Synthesis and Catalysis, 2012, 354, 2789-2796.	2.1	34
20	Delocalized Hole Domains in Guanine-Rich DNA Oligonucleotides. Journal of Physical Chemistry B, 2015, 119, 5462-5466.	1.2	33
21	Elementary electron transfer reactions: from basic concepts to recent computational advances. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 542-559.	6.2	32
22	Absorption Band Shapes of a Pushâ€“Pull Dye Approaching the Cyanine Limit: A Challenging Case for First Principle Calculations. Journal of Physical Chemistry A, 2016, 120, 5581-5589.	1.1	31
23	Hole Hopping Rates in Organic Semiconductors: A Second-Order Cumulant Approach. Journal of Chemical Theory and Computation, 2018, 14, 1594-1601.	2.3	31
24	Synthesis, spectroscopic properties and DFT calculations of a novel multipolar azo dye and its zinc(II) complex. Inorganic Chemistry Communication, 2017, 84, 103-108.	1.8	30
25	Second-Order Cumulant Approach for the Evaluation of Anisotropic Hole Mobility in Organic Semiconductors. Journal of Physical Chemistry C, 2018, 122, 25849-25857.	1.5	29
26	Quantitative Prediction of the Electroâ€Mechanical Response in Organic Crystals. Advanced Materials, 2021, 33, e2008049.	11.1	29
27	Title is missing!. Structural Chemistry, 2002, 13, 27-36.	1.0	28
28	Role of Intramolecular Vibrations in Long-Range Electron Transfer between Pheophytin and Ubiquinone in Bacterial Photosynthetic Reaction Centers. Biophysical Journal, 2005, 89, 830-841.	0.2	28
29	The Chargeâ€Transfer Band of an Oxidized Watsonâ€“Crick Guanosineâ€“Cytidine Complex. Angewandte Chemie - International Edition, 2009, 48, 9526-9528.	7.2	28
30	Tuning Wavefunction Mixing in Pushâ€“Pull Molecules: From Neutral to Zwitterionic Compounds. European Journal of Organic Chemistry, 2012, 2012, 2980-2989.	1.2	28
31	Molecular hyperpolarizabilities of pushâ€“pull chromophores: A comparison between theoretical and experimental results. Chemical Physics, 2013, 411, 11-16.	0.9	28
32	On the Occurrence of an Electron-Transfer Step in Aromatic Nitration. The Journal of Physical Chemistry, 1996, 100, 5303-5309.	2.9	27
33	Hole delocalization over adenine tracts in single stranded DNA oligonucleotides. Physical Chemistry Chemical Physics, 2015, 17, 4750-4756.	1.3	27
34	Tautomerism in the Fused NâRich TriÂazolotriazole Heterocyclic System. European Journal of Organic Chemistry, 2013, 2013, 3721-3728.	1.2	26
35	Enantioselective Conjugate Addition of Malononitrile to Chalcones Promoted by Î±,Î±â€‹scp›L‹/scp›â€Diaryl Prolinols: Noncovalent versus Covalent Catalysis?. European Journal of Organic Chemistry, 2011, 2011, 1922-1931.	1.2	25
36	The Dynamics of Hole Transfer in DNA. Molecules, 2019, 24, 4044.	1.7	25

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37	Stacking Interactions between Adenines in Oxidized Oligonucleotides. Journal of Physical Chemistry B, 2013, 117, 8947-8953.	1.2	24
38	Tuning optical absorption in pyran derivatives for DSSC. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 321, 79-89.	2.0	24
39	Vibronic couplings and coherent electron transfer in bridged systems. Physical Chemistry Chemical Physics, 2015, 17, 30937-30945.	1.3	23
40	Self-consistent-field calculations of the vibrational spectrum of undoped and doped transpolyacetylene. Canadian Journal of Chemistry, 1985, 63, 1553-1561.	0.6	22
41	An Anthracene-Incorporated [8]Cycloparaphenylene Derivative as an Emitter in Photon Upconversion. Journal of Organic Chemistry, 2018, 83, 220-227.	1.7	22
42	Explaining different experimental hole mobilities: influence of polymorphism on dynamic disorder in pentacene. Journal of Materials Chemistry C, 2019, 7, 9665-9670.	2.7	22
43	A theoretical analysis of excited state proton transfer in 3-hydroxyflavone. Promoting effect of a low frequency bending mode. Journal of Mathematical Chemistry, 1992, 10, 249-274.	0.7	21
44	Electron transfer rates and Franckâ€“Condon factors: an application to the early electron transfer steps in photosynthetic reaction centers. Theoretical Chemistry Accounts, 2007, 117, 957-967.	0.5	21
45	Novel pyran based dyes for application in dye sensitized solar cells. Dyes and Pigments, 2016, 133, 395-405.	2.0	21
46	Electron Transfer between Quinones in Photosynthetic Reaction Centers. Journal of Physical Chemistry B, 2004, 108, 3068-3077.	1.2	20
47	Quantum Dynamics of Radiationless Electronic Transitions Including Normal Modes Displacements and Duschinsky Rotations: A Second-Order Cumulant Approach. Journal of Chemical Theory and Computation, 2015, 11, 415-422.	2.3	19
48	Quantum dynamics of electronic transitions with Gauss-Hermite wave packets. Journal of Chemical Physics, 2016, 144, 114102.	1.2	19
49	Pushâ€“Pull Azoâ€Chromophores Containing Two Fused Pentatomic Heterocycles and Their Nonlinear Optical Properties. European Journal of Organic Chemistry, 2009, 2009, 3535-3543.	1.2	18
50	The oxidization potential of AA steps in single strand DNA oligomers. RSC Advances, 2014, 4, 47887-47893.	1.7	18
51	One-pot highly diastereoselective annulation to N-unprotected tetrasubstituted 2-pyrrolines. Green Chemistry, 2015, 17, 2137-2140.	4.6	18
52	Nâ€Rich Fused Heterocyclic Systems: Synthesis, Structure, Optical and Electrochemical Characterization. European Journal of Organic Chemistry, 2016, 2016, 1772-1780.	1.2	18
53	Different nonlinear optical performances of polymers containing benzimidazole chromophores. Optical Materials, 2007, 30, 473-477.	1.7	17
54	Transient and Enduring Electronic Resonances Drive Coherent Long Distance Charge Transport in Molecular Wires. Journal of Physical Chemistry Letters, 2019, 10, 1845-1851.	2.1	17

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55	An alternative way of thinking about electron transfer in proteins: Proton assisted electron transfer between the primary and the secondary quinones in photosynthetic reaction centers. Journal of Chemical Physics, 2000, 113, 3212-3218.	1.2	16
56	Competitive H-bonding synthons in organic hydrazides. CrystEngComm, 2010, 12, 1186-1193.	1.3	16
57	Proton transfer in oxidized adenosine self-aggregates. Journal of Chemical Physics, 2013, 139, 145101.	1.2	16
58	Modeling DNA oxidation in water. Physical Chemistry Chemical Physics, 2017, 19, 13571-13578.	1.3	16
59	Coherent Effects in Charge Transport in Molecular Wires: Toward a Unifying Picture of Long-Range Hole Transfer in DNA. Journal of Physical Chemistry Letters, 2020, 11, 7769-7775.	2.1	16
60	Hydrogen bridges and electron transfer in biomolecules. Study of a possible mechanism on a model chargeâ€“recombination system. Canadian Journal of Chemistry, 1985, 63, 1850-1856.	0.6	15
61	Proton-Assisted Electron Transfer. Journal of Physical Chemistry A, 1998, 102, 10333-10339.	1.1	15
62	Polar crystals in imines of 4-hydroxybenzohydrazide: a comparison between racemic and enantiomorphic crystals. CrystEngComm, 2013, 15, 3318.	1.3	15
63	Hole hopping rates in single strand oligonucleotides. Chemical Physics, 2014, 440, 25-30.	0.9	15
64	High-Energy-Density Materials: An Amphoteric N-Rich Bis(triazole) and Salts of Its Cationic and Anionic Species. Inorganic Chemistry, 2021, 60, 16213-16222.	1.9	15
65	The infrared and Raman spectrum of trans-polyacetylene: A self-consistent-field study. Solid State Communications, 1985, 53, 893-896.	0.9	14
66	The Influence of Back-Biting Interaction on the Polymerization of Conjugated Dienes in the Presence of Zieglerâ^'Natta Catalysts. Macromolecules, 1999, 32, 6852-6855.	2.2	14
67	The occurrence of electron transfer in aromatic nitration: dynamical aspects. Theoretical Chemistry Accounts, 2000, 104, 218-222.	0.5	14
68	Electro-optical properties from CC2 Calculations: A comparison between theoretical and experimental results. Chemical Physics Letters, 2013, 580, 126-129.	1.2	14
69	Solid State Separation and Isolation of Tautomers of Fused-Ring Triazolotriazoles. Journal of Organic Chemistry, 2017, 82, 5155-5161.	1.7	14
70	A model for proton-assisted electron transfer. Chemical Physics Letters, 1999, 299, 511-517.	1.2	13
71	Perturbative calculation of Franckâ€“Condon integrals: New hints for a rational implementation. Journal of Chemical Physics, 2008, 129, 064116.	1.2	13
72	Proton induced tautomeric switching in N-rich aromatics with tunable acid-base character. Journal of Molecular Structure, 2015, 1093, 119-124.	1.8	13

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73	Excited state intramolecular proton transfer in free base hemiporphyrazine. Chemical Physics Letters, 2002, 354, 160-164.	1.2	12
74	Single-Stranded DNA Oligonucleotides Retain Rise Coordinates Characteristic of Double Helices. Journal of Physical Chemistry B, 2018, 122, 7978-7989.	1.2	12
75	On the electronic states of macrocycles of the extended porphyrin family and their coordination compounds. Computational and Theoretical Chemistry, 1997, 390, 101-107.	1.5	11
76	Ring to open-chain transformation induced by selective metal coordination in a new dithiocarbazate ligand. Inorganica Chimica Acta, 2013, 404, 29-33.	1.2	11
77	DFT predictions of the oxidation potential of organic dyes for opto-electronic devices. Computational and Theoretical Chemistry, 2015, 1070, 68-75.	1.1	11
78	Proton Assisted Electron Transfer. Advances in Quantum Chemistry, 2000, 36, 301-322.	0.4	10
79	The Photophysics of Free-Base Hemiporphyrazine:Â A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 3926-3931.	1.1	10
80	Disentangling Electronic and Vibrational Effects in the Prediction of Band Shapes for Singletâ€“Triplet Transitions. Journal of Physical Chemistry C, 2019, 123, 14173-14179.	1.5	10
81	Bis(phosphine)nickelacyclopentane: an investigation by local spin density theory. Inorganic Chemistry, 1990, 29, 1544-1549.	1.9	9
82	Arterial aneurysms associated with intracranial dural arteriovenous fistulas: epidemiology, natural history, and management. A systematic review. Neurosurgical Review, 2019, 42, 277-285.	1.2	9
83	The role of the ironâ€“histidine bridge in the early steps of photosynthesis. Chemical Physics Letters, 2003, 369, 549-555.	1.2	8
84	First Principle Analysis of Charge Dissociation and Charge Recombination Processes in Organic Solar Cells. Journal of Physical Chemistry C, 2015, 119, 18870-18876.	1.5	8
85	First-Principle Calculations of the Band Shapes of Singletâ€“Triplet Transitions. Journal of Physical Chemistry C, 2016, 120, 24605-24614.	1.5	8
86	Solid State Selection between Nearly Isoenergetic Tautomeric Forms Driven by Right Hydrogen-Bonding Pairing. Crystal Growth and Design, 2018, 18, 6293-6301.	1.4	7
87	Tautomeric and conformational switching in a new versatile N-rich heterocyclic ligand. Dalton Transactions, 2020, 49, 14452-14462.	1.6	7
88	A theoretical study of ion selectivity of zeolitesâ€”application to chabazite. Journal of Physics and Chemistry of Solids, 1987, 48, 1-12.	1.9	6
89	Radiationless decay via ESIPT of the first excited singlet of the hemiporphyrazine. Chemical Physics, 1996, 204, 347-351.	0.9	6
90	The mechanism of Ziegler-Natta polymerization of 4-methyl-1,3-pentadiene: a theoretical study of the coordination step. Computational and Theoretical Chemistry, 1998, 426, 249-255.	1.5	6

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91	A Simple Method for Estimating Activation Energies of Proton-Transfer Reactionsâ€. Journal of Physical Chemistry A, 2002, 106, 7018-7025.	1.1	6
92	Total synthesis of ichthyotoxic macrolides from the skin of the marine mollusk Aplysia depilans. Phytochemistry Reviews, 2004, 3, 417-422.	3.1	6
93	A Plausible Mechanism of Electron Transfer between Quinones in Photosynthetic Reaction Centers. Journal of Theoretical Biology, 2000, 207, 101-105.	0.8	5
94	Intramolecular reorganization energies and Franckâ€“Condon integrals for ET from pheophytin to quinone in bacterial photosynthetic reaction centers. Chemical Physics Letters, 2005, 413, 210-215.	1.2	5
95	Detection of an ylide intermediate in the electrochemically-induced Stevens rearrangement of an ammonium salt by in situ UVâ€“vis spectroelectrochemistry. Electrochimica Acta, 2013, 92, 446-451.	2.6	5
96	The Time Scale of Electronic Resonance in Oxidized DNA as Modulated by Solvent Response: An MD/QM-MM Study. Molecules, 2021, 26, 5497.	1.7	5
97	Paper-Strip-Based Sensors for H2S Detection: A Proof-of-Principle Study. Sensors, 2022, 22, 3173.	2.1	5
98	Charge distributions and chemical effects. XLV. Graphite. Canadian Journal of Chemistry, 1988, 66, 2631-2633.	0.6	4
99	Co2 electron dissociation in the 18â€“46 eV range. A report of the O+ and Co+ abundances. International Journal of Mass Spectrometry and Ion Processes, 1989, 87, 41-50.	1.9	4
100	Chemical effects and surface properties: The nature of an adsorbed complex. International Journal of Quantum Chemistry, 1994, 49, 429-448.	1.0	4
101	PM3 study of the electronic spectra of some substituted aminocoumarins. Computational and Theoretical Chemistry, 1998, 426, 145-153.	1.5	4
102	Neutral mixed-valence organic monoradicals. Chemical Physics Letters, 1999, 313, 582-586.	1.2	4
103	On the influence of unsaturation on the macrolactonization of hydroxy fatty acids. Journal of Physical Organic Chemistry, 2009, 22, 978-985.	0.9	4
104	Towards “ab-initio” Computations of Electron Transfer Rates: the Early Electron Transfer Steps in Bacterial Photosynthetic Reaction Centers. Current Organic Chemistry, 2010, 14, 90-105.	0.9	4
105	The association constant of 5â€²,8-cyclo-2â€²-deoxyguanosine with cytidine. Frontiers in Chemistry, 2015, 3, 22.	1.8	4
106	Phototautomerism of triazolo-triazole scaffold. Journal of Molecular Structure, 2020, 1203, 127368.	1.8	4
107	Is Aromatic Nitration Spin Density Driven?. Chemistry, 2021, 3, 1286-1301.	0.9	4
108	A possible role of histidine residues in long-range electron transfer in proteins. Theoretical Chemistry Accounts, 2004, 111, 303-310.	0.5	3

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109	Reliable Predictions of Benzophenone Singletâ€“Triplet Transition Rates: A Second-Order Cumulant Approach. Journal of Physical Chemistry A, 2021, 125, 43-49.	1.1	3
110	{4-Bromo-2-[(2-{(ethylsulfanyl)[(2-oxidobenzylidene-ÎºO)amino-ÎºN]methylidene}hydrazinylidene-ÎºN1)methyl]phenolato-ÎºO}(ethanol-ÎºO Acta Crystallographica Section E: Structure Reports Online, 2013, 69, m362-m363.	0.2	2
111	Temperature regiocontrol of intramolecular cyclization of di-hydroxysecoacids. Organic and Biomolecular Chemistry, 2004, 2, 3425.	1.5	1
112	Crystal structures and photoluminescence properties of chromium(III) complexes with 2-thenoyltrifluoroacetone ligand. Journal of Molecular Structure, 2021, 1245, 131023.	1.8	1
113	An entire class of compounds forming polar crystals and showing single-crystal-to-single-crystal transitions between polar phases. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, s71-s71.	0.3	1
114	Strong overcrowding in dimethyl 2-(dimethylamino)terephthalate. Acta Crystallographica Section C: Crystal Structure Communications, 2008, 64, o420-o422.	0.4	0
115	Franckâ€“Condon factors in curvilinear coordinates: the photoelectron spectrum of ammonia. Highlights in Theoretical Chemistry, 2013, , 207-216.	0.0	0
116	Current Density and Spectroscopyâ€”A Themed Issue in Honor of Professor Riccardo Zanasi on the Occasion of His 70th Birthday. Chemistry, 2022, 4, 118-120.	0.9	0