Francoise Remacle

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Measurement and laser control of attosecond charge migration in ionized iodoacetylene. Science, 2015, 350, 790-795.	12.6	463
2	DNA computing circuits using libraries of DNAzyme subunits. Nature Nanotechnology, 2010, 5, 417-422.	31.5	412
3	An electronic time scale in chemistry. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 6793-6798.	7.1	354
4	Architectonic Quantum Dot Solids. Accounts of Chemical Research, 1999, 32, 415-423.	15.6	349
5	All-DNA finite-state automata with finite memory. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 21996-22001.	7.1	129
6	Complexes of DNA Bases and Gold Clusters Au3 and Au4 Involving Nonconventional Nâ^'H···Au Hydrogen Bonding. Nano Letters, 2005, 5, 735-739.	9.1	126
7	Intermolecular and Intramolecular Logic Gates. Journal of Physical Chemistry B, 2001, 105, 5589-5591.	2.6	124
8	Quantum Dots as Chemical Building Blocks: Elementary Theoretical Considerations. ChemPhysChem, 2001, 2, 20-36.	2.1	122
9	Laser Steered Ultrafast Quantum Dynamics of Electrons in LiH. Physical Review Letters, 2007, 99, 183902.	7.8	121
10	Structure and energetics of two- and three-dimensional neutral, cationic, and anionic gold clusters Au5⩽n⩽9Z (Z=0,±1). Journal of Chemical Physics, 2005, 122, 044304.	3.0	109
11	pH-Programmable DNA Logic Arrays Powered by Modular DNAzyme Libraries. Nano Letters, 2012, 12, 6049-6054.	9.1	105
12	Electrochemically Driven Sequential Machines: An Implementation of Copper Rotaxanes. Chemistry - A European Journal, 2009, 15, 1310-1313.	3.3	100
13	Complexes of DNA Bases and Watsonâ^ Crick Base Pairs with Small Neutral Gold Clusters. Journal of Physical Chemistry B, 2005, 109, 22746-22757.	2.6	96
14	Electronic Control of Site Selective Reactivity:Â A Model Combining Charge Migration and Dissociation. Journal of Physical Chemistry A, 1999, 103, 10149-10158.	2.5	89
15	The magic gold cluster Au ₂₀ . International Journal of Quantum Chemistry, 2007, 107, 2922-2934.	2.0	87
16	Pump and probe ultrafast electron dynamics in LiH: a computational study. New Journal of Physics, 2008, 10, 025019.	2.9	87
17	Logic reversibility and thermodynamic irreversibility demonstrated by DNAzyme-based Toffoli and Fredkin logic gates. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 21228-21233.	7.1	82
18	Information-theoretic analysis of phenotype changes in early stages of carcinogenesis. Proceedings of the United States of America, 2010, 107, 10324-10329.	7.1	81

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19	A full-adder based on reconfigurable DNA-hairpin inputs and DNAzyme computing modules. Chemical Science, 2014, 5, 3381.	7.4	80
20	Charge directed reactivity:. Chemical Physics Letters, 1998, 285, 25-33.	2.6	79
21	Molecule-Based Photonically Switched Half and Full Adder. Journal of Physical Chemistry A, 2006, 110, 177-184.	2.5	78
22	DNAzyme-based 2:1 and 4:1 multiplexers and 1:2 demultiplexer. Chemical Science, 2014, 5, 1074.	7.4	78
23	Trapping in competitive decay of degenerate states. Physics Letters, Section A: General, Atomic and Solid State Physics, 1990, 145, 265-268.	2.1	71
24	Three-gold clusters form nonconventional hydrogen bonds O–H⋯Au and N–H⋯Au with formamide and formic acid. Chemical Physics Letters, 2005, 404, 142-149.	2.6	70
25	miRNA and mRNA cancer signatures determined by analysis of expression levels in large cohorts of patients. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 19160-19165.	7.1	64
26	Hypoxia induces a phase transition within a kinase signaling network in cancer cells. Proceedings of the United States of America, 2013, 110, E1352-60.	7.1	61
27	Decay of high Rydberg states: A paradigm for intramolecular dynamics in a congested bound level structure coupled to a continuum. Journal of Chemical Physics, 1996, 104, 1399-1414.	3.0	57
28	Probing Ultrafast Purely Electronic Charge Migration in Small Peptides. Zeitschrift Fur Physikalische Chemie, 2007, 221, 647-661.	2.8	57
29	Charge migration in the bifunctional PENNA cation induced and probed by ultrafast ionization: a dynamical study. Journal of Physics B: Atomic, Molecular and Optical Physics, 2014, 47, 124011.	1.5	57
30	Protein Signaling Networks from Single Cell Fluctuations and Information Theory Profiling. Biophysical Journal, 2011, 100, 2378-2386.	0.5	55
31	Networks of Quantum Nanodots:Â The Role of Disorder in Modifying Electronic and Optical Properties. Journal of Physical Chemistry B, 1998, 102, 7727-7734.	2.6	53
32	Electronic Response of Assemblies of Designer Atoms:  The Metalâ^'Insulator Transition and the Role of Disorder. Journal of the American Chemical Society, 2000, 122, 4084-4091.	13.7	53
33	Localized electron dynamics in attosecond-pulse-excited molecular systems: Probing the time-dependent electron density by sudden photoionization. Physical Review A, 2012, 86, .	2.5	53
34	Glioblastoma cellular architectures are predicted through the characterization of two-cell interactions. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 6521-6526.	7.1	52
35	Intercommunication of DNA-Based Constitutional Dynamic Networks. Journal of the American Chemical Society, 2018, 140, 8721-8731.	13.7	52
36	Coherent Electronic Wave Packet Motion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mi mathvariant="normal">C</mml:mi </mml:mrow><mml:mrow><mml:mn>60</mml:mn></mml:mrow>by the Waveform and Polarization of Few-Cycle Laser Fields. Physical Review Letters, 2015, 114, 123004.</mml:mrow></mml:math 	7.8 sub> <td>51 l:mrow></td>	51 l:mrow>

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37	Quantum dot artificial solids: Understanding the static and dynamic role of size and packing disorder. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 6456-6459.	7.1	50
38	Thermometer ions for matrix-enhanced laser desorption/ionization internal energy calibration. Rapid Communications in Mass Spectrometry, 2003, 17, 1847-1854.	1.5	50
39	Gating the Conductivity of Arrays of Metallic Quantum Dots. Journal of Physical Chemistry B, 2003, 107, 13892-13901.	2.6	48
40	On the feasibility of an ultrafast purely electronic reorganization in lithium hydride. Chemical Physics, 2007, 338, 342-347.	1.9	48
41	Electronic wave packet motion in water dimer cation: A many electron description. Chemical Physics, 2009, 366, 129-138.	1.9	48
42	On the strong and selective isotope effect in the UV excitation of N ₂ with implications toward the nebula and Martian atmosphere. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6020-6025.	7.1	48
43	On a fundamental structure of gene networks in living cells. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 4702-4707.	7.1	48
44	Charge migration and control of site selective reactivity: The role of covalent and ionic states. Journal of Chemical Physics, 1999, 110, 5089-5099.	3.0	47
45	The transition from localized to collective electronic states in a silver quantum dots monolayer examined by nonlinear optical response. Chemical Physics Letters, 1998, 291, 453-458.	2.6	46
46	Towards a molecular logic machine. Journal of Chemical Physics, 2001, 114, 10239-10246.	3.0	45
47	On Spectroscopy, Control, and Molecular Information Processing. ChemPhysChem, 2002, 3, 43-51.	2.1	45
48	Electrical addressing of confined quantum systems for quasiclassical computation and finite state logic machines. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 5653-5658.	7.1	44
49	Angular-resolved Photoelectron Spectroscopy of Superatom Orbitals of Fullerenes. Physical Review Letters, 2012, 108, 173401.	7.8	43
50	Electrical transmission of molecular bridges. Chemical Physics Letters, 2004, 383, 537-543.	2.6	42
51	Nonconventional Hydrogen Bonding between Clusters of Gold and Hydrogen Fluoride. Journal of Physical Chemistry A, 2005, 109, 7309-7318.	2.5	42
52	All-optical digital logic: Full addition or subtraction on a three-state system. Physical Review A, 2006, 73, .	2.5	42
53	The gold-ammonia bonding patterns of neutral and charged complexes Aum0±1–(NH3)n. I. Bonding and charge alternation. Journal of Chemical Physics, 2007, 127, 194305.	3.0	42
54	Attosecond pumping of nonstationary electronic states of LiH: Charge shake-up and electron density distortion. Physical Review A, 2011, 83, .	2.5	42

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55	Consecutive feedback-driven constitutional dynamic networks. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 2843-2848.	7.1	42
56	Conductivity of 2-D Ag Quantum Dot Arrays:Â Computational Study of the Role of Size and Packing Disorder at Low Temperatures. Journal of Physical Chemistry B, 2002, 106, 4116-4126.	2.6	38
57	Ligand and Solvation Effects on the Electronic Properties of Au ₅₅ Clusters: A Density Functional Theory Study. Nano Letters, 2009, 9, 3007-3011.	9.1	38
58	On Electronic Properties of Assemblies of Quantum Nanodotsâ€. Journal of Physical Chemistry A, 2000, 104, 4739-4747.	2.5	37
59	Integrated logic circuits using single-atom transistors. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 13969-13972.	7.1	37
60	Ternary DNA computing using 3 × 3 multiplication matrices. Chemical Science, 2015, 6, 1288-1292.	7.4	37
61	Experimental and Theoretical Study of the Reactivity of Gold Nanoparticles Towards Benzimidazoleâ€2â€ylidene Ligands. Chemistry - A European Journal, 2016, 22, 10446-10458.	3.3	36
62	Vibrational computing: Simulation of a full adder by optimal control. Journal of Chemical Physics, 2008, 128, 064110.	3.0	35
63	Architecture with designer atoms: Simple theoretical considerations. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 553-558.	7.1	34
64	Pump and Probe of Ultrafast Charge Reorganization in Small Peptides: A Computational Study through Sudden Ionizations. Journal of Physical Chemistry A, 2013, 117, 10513-10525.	2.5	34
65	Ligand and Solvation Effects on the Structural and Electronic Properties of Small Gold Clusters. Journal of Physical Chemistry C, 2014, 118, 4362-4376.	3.1	34
66	Charge Redistribution Effects on the UV–Vis Spectra of Small Ligated Gold Clusters: a Computational Study. Journal of Physical Chemistry C, 2015, 119, 10969-10980.	3.1	33
67	Superexchange, Localized, and Domain-Localized Charge States for Intramolecular Electron Transfer in Large Molecules and in Arrays of Quantum Dots. Journal of Physical Chemistry B, 2001, 105, 2153-2162.	2.6	32
68	Transcending Binary Logic by Gating Three Coupled Quantum Dots. Nano Letters, 2007, 7, 2795-2799.	9.1	32
69	Stereocontrol of attosecond time-scale electron dynamics in ABCU using ultrafast laser pulses: a computational study. Physical Chemistry Chemical Physics, 2011, 13, 8331.	2.8	32
70	Rotational autoionization and interseries coupling of high Rydberg states by the anisotropy of the molecular core: The quantal long time evolution. Journal of Chemical Physics, 1996, 105, 4649-4663.	3.0	31
71	Imaging Transport Disorder in Conducting Arrays of Metallic Quantum Dots: An Experimental and Computational Study. Advanced Materials, 2002, 14, 124-128.	21.0	31
72	Logic implementations using a single nanoparticle–protein hybrid. Nature Nanotechnology, 2010, 5, 451-457.	31.5	31

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73	Quantum Phenomena in Nanomaterials: Coherent Superpositions of Fine Structure States in CdSe Nanocrystals at Room Temperature. Journal of Physical Chemistry C, 2019, 123, 31286-31293.	3.1	31
74	Prompt and delayed ionization of large molecules. Physics Letters, Section A: General, Atomic and Solid State Physics, 1993, 173, 284-287.	2.1	30
75	Unimolecular Reaction Dynamics from Kinetic Energy Release Distributions. 2. A Study of the Reaction C6H5Br+→ C6H5++ Br by the Maximum Entropy Method. The Journal of Physical Chemistry, 1996, 100, 8003-8007.	2.9	30
76	Logic gates using high Rydberg states. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 2973-2978.	7.1	29
77	Probing Rapidlyâ€lonizing Superâ€Atom Molecular Orbitals in C ₆₀ : A Computational and Femtosecond Photoelectron Spectroscopy Study. ChemPhysChem, 2013, 14, 3332-3340.	2.1	29
78	Control of electronic dynamics visualized by angularly resolved photoelectron spectra: A dynamical simulation with an IR pump and XUV attosecond-pulse-train probe. Physical Review A, 2014, 89, .	2.5	29
79	Extracting laws of decay in the femto–picosecond range from autocorrelation functions. Journal of Chemical Physics, 1989, 91, 4155-4168.	3.0	28
80	Does a dissociating molecule sample the available phase space. The Journal of Physical Chemistry, 1991, 95, 7124-7127.	2.9	28
81	The time scale for electronic reorganization upon sudden ionization of the water and water-methanol hydrogen bonded dimers and of the weakly bound NO dimer. Journal of Chemical Physics, 2006, 125, 133321.	3.0	28
82	The post-Born–Oppenheimer regime: dynamics of electronic motion in molecules by attosecond few-cycle spectroscopy. Physica Scripta, 2009, 80, 048101.	2.5	28
83	Bonding patterns of [Ag ₂ â€alanine] ^{0,±} hybrid complexes and the implementation of molecular logic gates. International Journal of Quantum Chemistry, 2010, 110, 2237-2246.	2.0	28
84	Unimolecular Dissociation from a Dense Set of States. The Journal of Physical Chemistry, 1996, 100, 7962-7971.	2.9	27
85	Electrical transport in saturated and conjugated molecular wires. Faraday Discussions, 2006, 131, 45-67.	3.2	27
86	A Density Functional Theory Calculation of the Electronic Properties of Several High-Spin and Low-Spin Iron(II) Pyrazolylborate Complexes. Inorganic Chemistry, 2008, 47, 4005-4014.	4.0	27
87	Personalized disease signatures through information-theoretic compaction of big cancer data. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 7694-7699.	7.1	27
88	Room-Temperature Inter-Dot Coherent Dynamics in Multilayer Quantum Dot Materials. Journal of Physical Chemistry C, 2020, 124, 16222-16231.	3.1	27
89	Time domain information from resonant Raman excitation profiles: A direct inversion by maximum entropy. Journal of Chemical Physics, 1993, 99, 4908-4925.	3.0	26
90	Unimolecular reaction dynamics from kinetic energy release distributions. III. A comparative study of the halogenobenzene cations. Journal of Chemical Physics, 1999, 110, 2911-2921.	3.0	26

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91	Convergence of Logic of Cellular Regulation in Different Premalignant Cells by an Information Theoretic Approach. BMC Systems Biology, 2011, 5, 42.	3.0	26
92	Molecular decision trees realized by ultrafast electronic spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17183-17188.	7.1	26
93	Parallel and Multivalued Logic by the Two-Dimensional Photon-Echo Response of a Rhodamine–DNA Complex. Journal of Physical Chemistry Letters, 2015, 6, 1714-1718.	4.6	26
94	Reconfigurable Logic Devices on a Single Dopant Atom—Operation up to a Full Adder by Using Electrical Spectroscopy. ChemPhysChem, 2009, 10, 162-173.	2.1	25
95	Ternary logic implemented on a single dopant atom field effect silicon transistor. Applied Physics Letters, 2010, 96, .	3.3	25
96	Metabolomic analysis of the green microalga Chlamydomonas reinhardtii cultivated under day/night conditions. Journal of Biotechnology, 2015, 215, 20-26.	3.8	25
97	Spatial and temporal control of populations, branching ratios, and electronic coherences in LiH by a single one-cycle infrared pulse. Physical Review A, 2017, 95, .	2.5	25
98	Continuous variables logic via coupled automata using a DNAzyme cascade with feedback. Chemical Science, 2017, 8, 2161-2168.	7.4	24
99	Where Ion Mobility and Molecular Dynamics Meet To Unravel the (Un)Folding Mechanisms of an Oligorotaxane Molecular Switch. ACS Nano, 2017, 11, 10253-10263.	14.6	24
100	Coherent electronic and nuclear dynamics in a rhodamine heterodimer–DNA supramolecular complex. Physical Chemistry Chemical Physics, 2017, 19, 23043-23051.	2.8	24
101	Quantum Nuclear Dynamics Pumped and Probed by Ultrafast Polarization Controlled Steering of a Coherent Electronic State in LiH. Journal of Physical Chemistry A, 2016, 120, 3343-3352.	2.5	23
102	All Optical Full Adder Based on Intramolecular Electronic Energy Transfer in the Rhodamineâ^'Azulene Bichromophoric System. Journal of Physical Chemistry C, 2008, 112, 15880-15885.	3.1	22
103	Fast Energy Transfer in CdSe Quantum Dot Layered Structures: Controlling Coupling with Covalent-Bond Organic Linkers. Journal of Physical Chemistry C, 2018, 122, 5753-5758.	3.1	22
104	Metabolic, Physiological, and Transcriptomics Analysis of Batch Cultures of the Green Microalga Chlamydomonas Grown on Different Acetate Concentrations. Cells, 2019, 8, 1367.	4.1	22
105	Rydberg states about dipolar cores: The quantum dynamics of the long-range anisotropic interaction. Physical Review A, 1996, 54, 4789-4801.	2.5	21
106	The determination of time cross correlation functions by inversion of Raman excitation profiles. Chemical Physics Letters, 1993, 205, 267-270.	2.6	20
107	The sequential exploration of phase space in selectively excited polyatomic molecules. Journal of Chemical Physics, 1993, 98, 2144-2159.	3.0	20
108	Molecular logic by optical spectroscopy with output transfer by charge migration along a peptide. Chemical Physics, 2002, 281, 363-372.	1.9	20

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109	Computational, Structural, and Mechanistic Analysis of the Electrochemically Driven Pirouetting Motion of a Copper Rotaxane. Journal of Physical Chemistry B, 2009, 113, 6219-6229.	2.6	20
110	Tuning the Properties of Pd Nanoclusters by Ligand Coatings: Electronic Structure Computations on Phosphine, Thiol, and Mixed Phosphine–Thiol Ligand Shells. Journal of Physical Chemistry C, 2014, 118, 9790-9800.	3.1	20
111	Time-dependent view of an isotope effect in electron-nuclear nonequilibrium dynamics with applications to N ₂ . Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5890-5895.	7.1	20
112	Unimolecular reaction dynamics from kinetic energy release distributions. IV. dissociation of the pyridine ion. International Journal of Mass Spectrometry, 1999, 185-187, 155-163.	1.5	19
113	Nanowiring by Molecules. Journal of Physical Chemistry B, 2004, 108, 18129-18134.	2.6	19
114	Quasiclassical computation. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 12091-12095.	7.1	19
115	Transition from SAMO to Rydberg State Ionization in C ₆₀ in Femtosecond Laser Fields. Journal of Physical Chemistry Letters, 2016, 7, 4677-4682.	4.6	19
116	DNA-based constitutional dynamic networks as functional modules for logic gates and computing circuit operations. Chemical Science, 2021, 12, 5473-5483.	7.4	19
117	Ultrafast geometrical reorganization of a methane cation upon sudden ionization: an isotope effect on electronic non-equilibrium quantum dynamics. Physical Chemistry Chemical Physics, 2021, 23, 12051-12059.	2.8	19
118	Configuration Interaction between Covalent and Ionic States in the Quantal and Semiclassical Limits with Application to Coherent and Hopping Charge Migration. Journal of Physical Chemistry A, 2000, 104, 2341-2350.	2.5	18
119	IR-UV Double-Resonance Photodissociation of Nitric Acid (HONO2) Viewed as Molecular Information Processing. Angewandte Chemie - International Edition, 2001, 40, 2512-2514.	13.8	18
120	Selective bond formation triggered by short optical pulses: quantum dynamics of a four-center ring closure. Physical Chemistry Chemical Physics, 2020, 22, 22302-22313.	2.8	18
121	Quantum effects in competitive unimolecular reactions. Chemical Physics, 1991, 153, 201-217.	1.9	17
122	Controlled full adder or subtractor by vibrational quantum computing. Physical Review A, 2009, 80, .	2.5	17
123	Ultrafast Predissociation Mechanism of the ¹ Î _u States of ¹⁴ N ₂ and Its Isotopomers upon Attosecond Excitation from the Ground State. Journal of Physical Chemistry A, 2012, 116, 11311-11318.	2.5	17
124	Magnetostructural effects in ligand stabilized Pd13 clusters: a density functional theory study. Nanoscale, 2012, 4, 4138.	5.6	17
125	Atomistic account of structural and dynamical changes induced by small binders in the double helix of a short DNA. Physical Chemistry Chemical Physics, 2014, 16, 14070-14082.	2.8	17
126	Physical aspects and quantitative theory of time resolved spectroscopy of high molecular Rydberg states. Journal of Chemical Physics, 1997, 107, 3382-3391.	3.0	16

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127	Decay Dynamics of the Predissociating High Rydberg States of NO. Journal of Physical Chemistry A, 1998, 102, 9507-9517.	2.5	16
128	Small Gold Clusters Au5â‰ ¤ â‰ 8 and Their Cationic and Anionic Cousins. Advances in Quantum Chemistry, 2004, 47, 423-464.	0.8	16
129	Interplay of structural and electronic stabilizing factors in neutral and cationic phosphine protected Au13 clusters. European Physical Journal D, 2012, 66, 1.	1.3	16
130	Hot electron production and diffuse excited states in C70, C82, and Sc3N@C80 characterized by angular-resolved photoelectron spectroscopy. Journal of Chemical Physics, 2013, 139, 084309.	3.0	16
131	Nuclear Motion Driven Ultrafast Photodissociative Charge Transfer of the PENNA Cation: An Experimental and Computational Study. Journal of Physical Chemistry A, 2017, 121, 1442-1447.	2.5	16
132	Temporal and spatially resolved imaging of the correlated nuclear-electronic dynamics and of the ionized photoelectron in a coherently electronically highly excited vibrating LiH molecule. Journal of Chemical Physics, 2019, 151, 134310.	3.0	16
133	Angle-resolved photoelectron spectroscopy and scanning tunnelling spectroscopy studies of the endohedral fullerene Li@C ₆₀ . Nanoscale, 2019, 11, 2668-2678.	5.6	16
134	Quantum Device Emulates the Dynamics of Two Coupled Oscillators. Journal of Physical Chemistry Letters, 2020, 11, 6990-6995.	4.6	16
135	Current-voltage-temperature characteristics for 2D arrays of metallic quantum dots. Israel Journal of Chemistry, 2002, 42, 269-280.	2.3	15
136	A new electron-ion coincidence 3D momentum-imaging method and its application in probing strong field dynamics of 2-phenylethyl-N, N-dimethylamine. Journal of Chemical Physics, 2017, 147, 013920.	3.0	15
137	Electric Field Effects on Long Living ZEKE States. The Journal of Physical Chemistry, 1996, 100, 15320-15327.	2.9	14
138	On the inverse Born-Oppenheimer separation for high Rydberg states of molecules. International Journal of Quantum Chemistry, 1998, 67, 85-100.	2.0	14
139	Electronâ^'Nuclear Coupling in the Classical Limit for the Electronic Degrees of Freedomâ€. Journal of Physical Chemistry A, 2001, 105, 2708-2715.	2.5	14
140	A Counter Based on the Electrical Input/Output Stimuli Activation of an Array of Quantum Dots. ChemPhysChem, 2005, 6, 1239-1242.	2.1	14
141	Logic operations in a doped solid driven by stimulated Raman adiabatic passage. Physical Review A, 2011, 83, .	2.5	14
142	Stabilization of merocyanine by protonation, charge, and external electric fields and effects on the isomerization of spiropyran: a computational study. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	14
143	Electronic Dynamics by Ultrafast Pump Photoelectron Detachment Probed by Ionization: A Dynamical Simulation of Negative–Neutral–Positive in LiH [–] . Journal of Physical Chemistry A, 2014, 118, 6721-6729.	2.5	14
144	On the quantum mechanical theory of unimolecular reactions through a narrow bottleneck: the prompt and delayed dissociation. Molecular Physics, 1996, 87, 899-917.	1.7	13

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145	Prompt and Delayed Dissociation of Energy-Rich Larger Molecules. Journal of Physical Chemistry A, 1998, 102, 10195-10198.	2.5	13
146	Size Effects in the Electronic Properties of Finite Arrays of Exchange-Coupled Quantum Dots. Journal of Physical Chemistry B, 2002, 106, 12847-12850.	2.6	13
147	Thiophenol and thiophenol radical and their complexes with gold clusters Au5 and Au6. Journal of Molecular Structure, 2004, 708, 165-173.	3.6	13
148	Controlled full adder–subtractor by vibrational computing. Physical Chemistry Chemical Physics, 2010, 12, 15628.	2.8	13
149	Surprisal Analysis of Glioblastoma Multiform (GBM) MicroRNA Dynamics Unveils Tumor Specific Phenotype. PLoS ONE, 2014, 9, e108171.	2.5	13
150	Relative Photoionization Cross Sections of Super-Atom Molecular Orbitals (SAMOs) in C ₆₀ . Journal of Physical Chemistry A, 2015, 119, 11504-11508.	2.5	13
151	Probing in Space and Time the Nuclear Motion Driven by Nonequilibrium Electronic Dynamics in Ultrafast Pumped N ₂ . Journal of Physical Chemistry A, 2016, 120, 3335-3342.	2.5	13
152	Low-lying, Rydberg states of polycyclic aromatic hydrocarbons (PAHs) and cyclic alkanes. Physical Chemistry Chemical Physics, 2017, 19, 24090-24099.	2.8	13
153	Ultrafast 25-fs relaxation in highly excited states of methyl azide mediated by strong nonadiabatic coupling. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E11072-E11081.	7.1	13
154	Ultrafast fs coherent excitonic dynamics in CdSe quantum dots assemblies addressed and probed by 2D electronic spectroscopy. Journal of Chemical Physics, 2021, 154, 014301.	3.0	13
155	The maximum entropy of an optical spectrum and the redistribution in phase space. Chemical Physics Letters, 1991, 181, 307-311.	2.6	12
156	Broken Symmetry in the Density of Electronic States of an Array of Quantum Dots As Computed for Scanning Tunneling Microscopyâ€. Journal of Physical Chemistry A, 2000, 104, 10435-10441.	2.5	12
157	Level crossing conductance spectroscopy of molecular bridges. Applied Physics Letters, 2004, 85, 1725-1727.	3.3	12
158	Principles of design of a set-reset finite state logic nanomachine. Journal of Applied Physics, 2008, 104,	2.5	12
159	Combined Mössbauer Spectral and Density Functional Theory Determination of the Magnetic Easy-Axis in Two High-Spin Iron(II) 2-Pyrazinecarboxylate Complexes. Inorganic Chemistry, 2009, 48, 8173-8179.	4.0	12
160	Maximal entropy inference of oncogenicity from phosphorylation signaling. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 6112-6117.	7.1	12
161	DFT Studies of Solvation Effects on the Nanosize Bare, Thiolated, and Redox Active Ligated Au ₅₅ Cluster. Journal of Physical Chemistry C, 2010, 114, 15941-15950.	3.1	12
162	Electronic states and wavefunctions of diatomic donor molecular ions in silicon: multi-valley envelope function theory. Journal of Physics Condensed Matter, 2014, 26, 065302.	1.8	12

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163	Multivalley envelope function equations and effective potentials for phosphorus impurity in silicon. Physical Review B, 2015, 92, .	3.2	12
164	Coherent Exciton Dynamics in Ensembles of Size-Dispersed CdSe Quantum Dot Dimers Probed via Ultrafast Spectroscopy: A Quantum Computational Study. Applied Sciences (Switzerland), 2020, 10, 1328.	2.5	12
165	Electronic Isomerism: Symmetry Breaking and Electronic Phase Diagrams for Diatomic Molecules at the Large-Dimension Limit. ChemPhysChem, 2001, 2, 434-442.	2.1	11
166	Time-Resolved Electrochemical Spectroscopy of Charge Migration in Molecular Wires:  Computational Evidence for Rich Electronic Dynamics. Journal of Physical Chemistry C, 2007, 111, 2301-2309.	3.1	11
167	Ultrafast vibrational spectroscopy and relaxation in polyatomic molecules: Potential for molecular parallel computing. Chemical Physics, 2008, 347, 531-545.	1.9	11
168	AttoPhotoChemistry. Probing ultrafast electron dynamics by the induced nuclear motion: The prompt and delayed predissociation of N2. Chemical Physics Letters, 2014, 601, 45-48.	2.6	11
169	Computational Benchmarking for Ultrafast Electron Dynamics: Wave Function Methods vs Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 2221-2233.	5.3	11
170	Force measurements reveal how small binders perturb the dissociation mechanisms of DNA duplex sequences. Nanoscale, 2016, 8, 11718-11726.	5.6	11
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