Kenneth Lopata

List of Publications by Year
in descending order

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45	2,111	331670	233421
papers	citations	21 h-index	45 g-index

46	46	46	2280
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Intruder Peak-Free Transient Inner-Shell Spectra Using Real-Time Simulations. Journal of Chemical Theory and Computation, 2022, 18, 992-1002.	5.3	5
2	Charge migration and attosecond solitons in conjugated organic molecules. Physical Review Research, 2022, 4, .	3.6	17
3	Characterizing particle-like charge-migration dynamics with high-order harmonic sideband spectroscopy. Physical Review A, 2022, 106, .	2.5	4
4	Mapping static core-holes and ring-currents with X-ray scattering. Faraday Discussions, 2021, 228, 60-81.	3.2	14
5	Strong-field induced fragmentation and isomerization of toluene probed by ultrafast femtosecond electron diffraction and mass spectrometry. Faraday Discussions, 2021, 228, 39-59.	3.2	10
6	Molecular Modes of Attosecond Charge Migration. Physical Review Letters, 2021, 126, 133002.	7.8	38
7	Orbital-resolved calculations of two-center interferences in linear triatomic molecules. Physical Review A, 2021, 104, .	2.5	5
8	Time-resolved diffraction: general discussion. Faraday Discussions, 2021, 228, 161-190.	3.2	2
9	Growth Dynamics of Colloidal Silverâ€“Gold Coreâ€“Shell Nanoparticles Studied by In Situ Second Harmonic Generation and Extinction Spectroscopy. Journal of Physical Chemistry C, 2021, 125, 25615-25623.	3.1	7
10	Simulated field-modulated x-ray absorption in titania. Journal of Chemical Physics, 2020, 153, 054110.	3.0	5
11	Multidimensional molecular high-harmonic spectroscopy: A road map for charge migration studies. Journal of Molecular Spectroscopy, 2020, 372, 111353.	1.2	16
12	Real-Time Time-Dependent Electronic Structure Theory. Chemical Reviews, 2020, 120, 9951-9993.	47.7	141
13	First-Principles Simulations of X-ray Transient Absorption for Probing Attosecond Electron Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 4470-4478.	5.3	22
14	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
15	Integral Representation of Weak-Field Asymptotic Theory using Density Functional Orbitals and Potentials for an Efficient and Qualitatively Accurate Calculation of Angle Dependent Ionization Rate. , 2020, , .		0
16	High-harmonic spectroscopy of transient two-center interference calculated with time-dependent density-functional theory. Structural Dynamics, 2019, 6, 044101.	2.3	10
17	Probing the interplay between geometric and electronic-structure features via high-harmonic spectroscopy. Journal of Chemical Physics, 2019, 150, 184308.	3.0	14
18	Angle-dependent strong-field ionization of halomethanes. Journal of Chemical Physics, 2019, 151, 194308.	3.0	30

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19	Monitoring the growth dynamics of colloidal gold-silver core-shell nanoparticles using in situ second harmonic generation and extinction spectroscopy. Journal of Chemical Physics, 2019, 151, 224701.	3.0	11
20	Wavelength and intensity dependence of recollision-enhanced multielectron effects in high-order harmonic generation. Physical Review A, 2018, 97, .	2.5	8
21	Signature of charge migration in modulations of double ionization. Physical Review A, 2018, 97, .	2.5	5
22	Angle dependence of strong-field single and double ionization of carbonyl sulfide. Physical Review A, 2018, 98, .	2.5	41
23	Capturing Plasmonâ€“Molecule Dynamics in Dye Monolayers on Metal Nanoparticles Using Classical Electrodynamics with Quantum Embedding. Journal of Physical Chemistry C, 2017, 121, 16932-16942.	3.1	16
24	Attosecond Charge Migration with TDDFT: Accurate Dynamics from a Well-Defined Initial State. Journal of Physical Chemistry Letters, 2017, 8, 3991-3996.	4.6	66
25	Angle-dependent strong-field molecular ionization rates with tuned range-separated time-dependent density functional theory. Journal of Chemical Physics, 2016, 145, 094105.	3.0	38
26	Semiclassical-wave-function perspective on high-harmonic generation. Physical Review A, 2016, 93, .	2.5	7
27	Accelerated Broadband Spectra Using Transition Dipole Decomposition and PadÃ© Approximants. Journal of Chemical Theory and Computation, 2016, 12, 3741-3750.	5.3	86
28	Comparison of Real-Time and Linear-Response Time-Dependent Density Functional Theories for Molecular Chromophores Ranging from Sparse to High Densities of States. Journal of Chemical Theory and Computation, 2015, 11, 1102-1109.	5.3	98
29	X-ray Absorption in Insulators with Non-Hermitian Real-Time Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 646-654.	5.3	38
30	Near and Above Ionization Electronic Excitations with Non-Hermitian Real-Time Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 4939-4946.	5.3	48
31	Optical Absorption and Band Gap Reduction in (Fe1â€“xCrx)2O3 Solid Solutions: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 25504-25512.	3.1	43
32	Optical absorption and spectral photoconductivity in Î±-(Fe_{1â€“x}Cr_x)₂O₃ solid-solution thin films. Journal of Physics Condensed Matter, 2013, 25, 392002.	1.8	33
33	Linear-Response and Real-Time Time-Dependent Density Functional Theory Studies of Core-Level Near-Edge X-Ray Absorption. Journal of Chemical Theory and Computation, 2012, 8, 3284-3292.	5.3	192
34	Electron transfer beyond the static picture: A TDDFT/TD-ZINDO study of a pentacene dimer. Journal of Chemical Physics, 2012, 137, 22A502.	3.0	11
35	A Combined Gasâ€Phase Photoelectron Spectroscopic and Theoretical Study of Zeiseâ€™s Anion and Its Bromine and Iodine Analogues. Angewandte Chemie - International Edition, 2012, 51, 6356-6360.	13.8	11
36	Modeling molecular effects on plasmon transport: Silver nanoparticles with tartrazine. Journal of Chemical Physics, 2011, 134, 084101.	3.0	18

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37	Visible Light Absorption of N-Doped TiO₂ Rutile Using (LR/RT)-TDDFT and Active Space EOMCCSD Calculations. Journal of Physical Chemistry Letters, 2011, 2, 2696-2701.	4.6	26
38	Excited-State Studies of Polyacenes: A Comparative Picture Using EOMCCSD, CR-EOMCCSD(T), Range-Separated (LR/RT)-TDDFT, TD-PM3, and TD-ZINDO. Journal of Chemical Theory and Computation, 2011, 7, 3686-3693.	5.3	84
39	Modeling Fast Electron Dynamics with Real-Time Time-Dependent Density Functional Theory: Application to Small Molecules and Chromophores. Journal of Chemical Theory and Computation, 2011, 7, 1344-1355.	5.3	217
40	Graphene nanomeshes: Onset of conduction band gaps. Chemical Physics Letters, 2010, 498, 334-337.	2.6	27
41	Nonlinear nanopolaritonics: Finite-difference time-domain Maxwellâ€“SchrÃ¶dinger simulation of molecule-assisted plasmon transfer. Journal of Chemical Physics, 2009, 131, 014701.	3.0	51
42	Multiscale Maxwellâ€“SchrÃ¶dinger modeling: A split field finite-difference time-domain approach to molecular nanopolaritonics. Journal of Chemical Physics, 2009, 130, 104707.	3.0	84
43	Quantum Drude friction for time-dependent density functional theory. Journal of Chemical Physics, 2008, 129, 134106.	3.0	16
44	Curve crossing and negative refraction in simulations of near-field coupled metallic nanoparticle arrays. Journal of Chemical Physics, 2007, 127, 154714.	3.0	11
45	Molecular nanopolaritonics: Cross manipulation of near-field plasmons and molecules. I. Theory and application to junction control. Journal of Chemical Physics, 2007, 127, 154715.	3.0	59