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	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
2	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
3	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
4	Real-Time Time-Dependent Electronic Structure Theory. Chemical Reviews, 2020, 120, 9951-9993.	47.7	141
5	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
6	Accelerated Broadband Spectra Using Transition Dipole Decomposition and PadÃ© Approximants. Journal of Chemical Theory and Computation, 2016, 12, 3741-3750.	5.3	86
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	Angle dependence of strong-field single and double ionization of carbonyl sulfide. Physical Review A, 2018, 98, .	2.5	41
15	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
16	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
17	Molecular Modes of Attosecond Charge Migration. Physical Review Letters, 2021, 126, 133002.	7.8	38
18	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

#	Article	IF	Citations
19	Angle-dependent strong-field ionization of halomethanes. Journal of Chemical Physics, 2019, 151, 194308.	3.0	30
20	Graphene nanomeshes: Onset of conduction band gaps. Chemical Physics Letters, 2010, 498, 334-337.	2.6	27
21	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
22	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
23	Modeling molecular effects on plasmon transport: Silver nanoparticles with tartrazine. Journal of Chemical Physics, 2011, 134, 084101.	3.0	18
24	Charge migration and attosecond solitons in conjugated organic molecules. Physical Review Research, 2022, 4, .	3.6	17
25	Quantum Drude friction for time-dependent density functional theory. Journal of Chemical Physics, 2008, 129, 134106.	3.0	16
26	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
27	Multidimensional molecular high-harmonic spectroscopy: A road map for charge migration studies. Journal of Molecular Spectroscopy, 2020, 372, 111353.	1.2	16
28	Probing the interplay between geometric and electronic-structure features via high-harmonic spectroscopy. Journal of Chemical Physics, 2019, 150, 184308.	3.0	14
29	Mapping static core-holes and ring-currents with X-ray scattering. Faraday Discussions, 2021, 228, 60-81.	3.2	14
30	Curve crossing and negative refraction in simulations of near-field coupled metallic nanoparticle arrays. Journal of Chemical Physics, 2007, 127, 154714.	3.0	11
31	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
32	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
33	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
34	High-harmonic spectroscopy of transient two-center interference calculated with time-dependent density-functional theory. Structural Dynamics, 2019, 6, 044101.	2.3	10
35	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
36	Wavelength and intensity dependence of recollision-enhanced multielectron effects in high-order harmonic generation. Physical Review A, 2018, 97, .	2.5	8

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37	Semiclassical-wave-function perspective on high-harmonic generation. Physical Review A, 2016, 93, .	2.5	7
38	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
39	Signature of charge migration in modulations of double ionization. Physical Review A, 2018, 97, .	2.5	5
40	Simulated field-modulated x-ray absorption in titania. Journal of Chemical Physics, 2020, 153, 054110.	3.0	5
41	Orbital-resolved calculations of two-center interferences in linear triatomic molecules. Physical Review A, 2021, 104, .	2.5	5
42	Intruder Peak-Free Transient Inner-Shell Spectra Using Real-Time Simulations. Journal of Chemical Theory and Computation, 2022, 18, 992-1002.	5.3	5
43	Characterizing particle-like charge-migration dynamics with high-order harmonic sideband spectroscopy. Physical Review A, 2022, 106, .	2.5	4
44	Time-resolved diffraction: general discussion. Faraday Discussions, 2021, 228, 161-190.	3.2	2
45	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