C William Mccurdy

List of Publications by Year
in descending order

37 papers	1,973 citations	279798 23 h-index	330143 37 g-index
39 all docs	39 docs citations	39 times ranked	1296 citing authors

#	Article	IF	Citations
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
2	What will it take to observe processes in 'real time'?. Nature Photonics, 2014, 8, 162-166.	31.4	220
3	Wave packet formulation of the boomerang model for resonant electronâ€“molecule scattering. Journal of Chemical Physics, 1983, 78, 6773-6779.	3.0	116
4	Applicability of selfâ€consistent field techniques based on the complex coordinate method to metastable electronic states. Journal of Chemical Physics, 1980, 73, 3268-3273.	3.0	91
5	Interrelation between variational principles for scattering amplitudes and generalizedR-matrix theory. Physical Review A, 1987, 36, 2061-2066.	2.5	87
6	Collisions of electrons with polyatomic molecules: Electron-methane scattering by the complex Kohn variational method. Physical Review A, 1989, 39, 4487-4493.	2.5	81
7	Implementation of exterior complex scaling in B-splines to solve atomic and molecular collision problems. Journal of Physics B: Atomic, Molecular and Optical Physics, 2004, 37, 917-936.	1.5	75
8	Solving the time-dependent SchrÃ¶dinger equation using complex-coordinate contours. Physical Review A, 1991, 43, 5980-5990.	2.5	58
9	Complex potential-energy function for theÎ£u+2shape resonance state ofH2â^'at the self-consistent-field level. Physical Review A, 1982, 25, 2529-2538.	2.5	55
10	High-spectral-resolution attosecond absorption spectroscopy of autoionization in xenon. Physical Review A, 2014, 89, .	2.5	54
11	Eliminating wavepacket reflection from grid boundaries using complex coordinate contours. Computer Physics Communications, 1991, 63, 323-330.	7.5	53
12	Practical calculation of amplitudes for electron-impact ionization. Physical Review A, 2001, 63, .	2.5	50
13	Complex basis functions revisited: Implementation with applications to carbon tetrafluoride and aromatic N-containing heterocycles within the static-exchange approximation. Journal of Chemical Physics, 2015, 142, 054103.	3.0	46
14	Feshbach resonances in electronâ€“molecule scattering by the complex multiconfiguration SCF and configuration interaction procedures: The 1Î£+g autoionizing states of H2. Journal of Chemical Physics, 1985, 83, 3547-3559.	3.0	45
15	Electronic excitation ofH2by electron impact: Close-coupling calculations using the complex Kohn variational method. Physical Review A, 1991, 43, 3514-3521.	2.5	44
16	Angular dependence of dissociative electron attachment to polyatomic molecules: Application to theB12metastable state of theH2OandH2Sanions. Physical Review A, 2006, 73, .	2.5	42
17	Conversion of bound states to resonances with changing internuclear distance in molecular anions. Journal of Chemical Physics, 1983, 79, 2200-2205.	3.0	38
18	Time-dependent approach to collisional ionization using exterior complex scaling. Physical Review A, 2002, 65, .	2.5	36

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19	Second order MÃ¸ller-Plesset and coupled cluster singles and doubles methods with complex basis functions for resonances in electron-molecule scattering. Journal of Chemical Physics, 2017, 146, 234107.	3.0	36
20	Restricted and unrestricted non-Hermitian Hartree-Fock: Theory, practical considerations, and applications to metastable molecular anions. Journal of Chemical Physics, 2015, 143, 074103.	3.0	31
21	Probing autoionizing states of molecular oxygen with XUV transient absorption: Electronic-symmetry-dependent line shapes and laser-induced modifications. Physical Review A, 2017, 95, .	2.5	28
22	Progress in the application of classicalSâ€matrix theory to inelastic collision processes. Journal of Chemical Physics, 1980, 73, 3191-3197.	3.0	26
23	Electron-helium scattering in theS-wave model using exterior complex scaling. Physical Review A, 2005, 71, .	2.5	24
24	Three-body breakup in dissociative electron attachment to the water molecule. Physical Review A, 2008, 78, .	2.5	16
25	Stabilizing potentials in bound state analytic continuation methods for electronic resonances in polyatomic molecules. Journal of Chemical Physics, 2017, 146, 044112.	3.0	16
26	Investigation of coupling mechanisms in attosecond transient absorption of autoionizing states: comparison of theory and experiment in xenon. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 125601.	1.5	14
27	Ultrafast Rydberg-state dissociation in oxygen: Identifying the role of multielectron excitations. Physical Review A, 2019, 99, .	2.5	11
28	Coupled nuclearâ€“electronic decay dynamics of O₂ inner valence excited states revealed by attosecond XUV wave-mixing spectroscopy. Faraday Discussions, 2021, 228, 537-554.	3.2	11
29	Ultrafast photodissociation dynamics and nonadiabatic coupling between excited electronic states of methanol probed by time-resolved photoelectron spectroscopy. Journal of Chemical Physics, 2019, 150, 114301.	3.0	10
30	Validity of the isolated resonance picture forH2autoionizing states. Physical Review A, 2006, 73, .	2.5	9
31	Variational treatment of electronâ€“polyatomic-molecule scattering calculations using adaptive overset grids. Physical Review A, 2017, 96, .	2.5	8
32	Correlated variational treatment of ionization coupled to nuclear motion: Ultrafast pump and ionizing probe of electronic and nuclear dynamics in LiH. Physical Review Research, 2021, 3, .	3.6	7
33	Construction of complex STO-NG basis sets by the method of least squares and their applications. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	6
34	Dissociative recombination by frame transformation to Siegert pseudostates: A comparison with a numerically solvable model. Physical Review A, 2018, 97, .	2.5	5
35	Validity of the static-exchange approximation for inner-shell photoionization of polyatomic molecules. Physical Review A, 2020, 102, .	2.5	4
36	Two-photon double photoionization of atomic Mg by ultrashort pulses: Variation of angular distributions with pulse length. Physical Review A, 2020, 102, .	2.5	1

#	Article	IF	Citations
37	Exploring spin symmetry-breaking effects for static field ionization of atoms: Is there an analog to the Coulsonâ€“Fischer point in bond dissociation?. Journal of Chemical Physics, 2021, 155, 014309.	3.0	1