

C William Mccurdy

List of Publications by Year in descending order

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37
papers

1,973
citations

279798

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#	ARTICLE	IF	CITATIONS
1	Coupled nuclearâ€“electronic decay dynamics of O_{2} inner valence excited states revealed by attosecond XUV wave-mixing spectroscopy. <i>Faraday Discussions</i> , 2021, 228, 537-554.	3.2	11
2	Correlated variational treatment of ionization coupled to nuclear motion: Ultrafast pump and ionizing probe of electronic and nuclear dynamics in LiH. <i>Physical Review Research</i> , 2021, 3, .	3.6	7
3	Exploring spin symmetry-breaking effects for static field ionization of atoms: Is there an analog to the Coulsonâ€“Fischer point in bond dissociation?. <i>Journal of Chemical Physics</i> , 2021, 155, 014309.	3.0	1
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	3.0	518
5	Validity of the static-exchange approximation for inner-shell photoionization of polyatomic molecules. <i>Physical Review A</i> , 2020, 102, .	2.5	4
6	Two-photon double photoionization of atomic Mg by ultrashort pulses: Variation of angular distributions with pulse length. <i>Physical Review A</i> , 2020, 102, .	2.5	1
7	Ultrafast Rydberg-state dissociation in oxygen: Identifying the role of multielectron excitations. <i>Physical Review A</i> , 2019, 99, .	2.5	11
8	Ultrafast photodissociation dynamics and nonadiabatic coupling between excited electronic states of methanol probed by time-resolved photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , 2019, 150, 114301.	3.0	10
9	Dissociative recombination by frame transformation to Siegert pseudostates: A comparison with a numerically solvable model. <i>Physical Review A</i> , 2018, 97, .	2.5	5
10	Stabilizing potentials in bound state analytic continuation methods for electronic resonances in polyatomic molecules. <i>Journal of Chemical Physics</i> , 2017, 146, 044112.	3.0	16
11	Second order MÅller-Plesset and coupled cluster singles and doubles methods with complex basis functions for resonances in electron-molecule scattering. <i>Journal of Chemical Physics</i> , 2017, 146, 234107.	3.0	36
12	Probing autoionizing states of molecular oxygen with XUV transient absorption: Electronic-symmetry-dependent line shapes and laser-induced modifications. <i>Physical Review A</i> , 2017, 95, .	2.5	28
13	Variational treatment of electronâ€“polyatomic-molecule scattering calculations using adaptive overset grids. <i>Physical Review A</i> , 2017, 96, .	2.5	8
14	Restricted and unrestricted non-Hermitian Hartree-Fock: Theory, practical considerations, and applications to metastable molecular anions. <i>Journal of Chemical Physics</i> , 2015, 143, 074103.	3.0	31
15	Investigation of coupling mechanisms in attosecond transient absorption of autoionizing states: comparison of theory and experiment in xenon. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2015, 48, 125601.	1.5	14
16	Complex basis functions revisited: Implementation with applications to carbon tetrafluoride and aromatic N-containing heterocycles within the static-exchange approximation. <i>Journal of Chemical Physics</i> , 2015, 142, 054103.	3.0	46
17	High-spectral-resolution attosecond absorption spectroscopy of autoionization in xenon. <i>Physical Review A</i> , 2014, 89, .	2.5	54
18	What will it take to observe processes in 'real time'?. <i>Nature Photonics</i> , 2014, 8, 162-166.	31.4	220

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19	Construction of complex STO-NG basis sets by the method of least squares and their applications. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	6
20	Three-body breakup in dissociative electron attachment to the water molecule. <i>Physical Review A</i> , 2008, 78, .	2.5	16
21	Validity of the isolated resonance picture for H ₂ autoionizing states. <i>Physical Review A</i> , 2006, 73, .	2.5	9
22	Angular dependence of dissociative electron attachment to polyatomic molecules: Application to the B ¹ Σ ⁺ metastable state of the H ₂ O and H ₂ S anions. <i>Physical Review A</i> , 2006, 73, .	2.5	42
23	Electron-helium scattering in the S-wave model using exterior complex scaling. <i>Physical Review A</i> , 2005, 71, .	2.5	24
24	Implementation of exterior complex scaling in B-splines to solve atomic and molecular collision problems. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2004, 37, 917-936.	1.5	75
25	Time-dependent approach to collisional ionization using exterior complex scaling. <i>Physical Review A</i> , 2002, 65, .	2.5	36
26	Practical calculation of amplitudes for electron-impact ionization. <i>Physical Review A</i> , 2001, 63, .	2.5	50
27	Eliminating wavepacket reflection from grid boundaries using complex coordinate contours. <i>Computer Physics Communications</i> , 1991, 63, 323-330.	7.5	53
28	Solving the time-dependent Schrödinger equation using complex-coordinate contours. <i>Physical Review A</i> , 1991, 43, 5980-5990.	2.5	58
29	Electronic excitation of H ₂ by electron impact: Close-coupling calculations using the complex Kohn variational method. <i>Physical Review A</i> , 1991, 43, 3514-3521.	2.5	44
30	Collisions of electrons with polyatomic molecules: Electron-methane scattering by the complex Kohn variational method. <i>Physical Review A</i> , 1989, 39, 4487-4493.	2.5	81
31	Interrelation between variational principles for scattering amplitudes and generalized R-matrix theory. <i>Physical Review A</i> , 1987, 36, 2061-2066.	2.5	87
32	Feshbach resonances in electron-molecule scattering by the complex multiconfiguration SCF and configuration interaction procedures: The 1 ¹ Σ ⁺ autoionizing states of H ₂ . <i>Journal of Chemical Physics</i> , 1985, 83, 3547-3559.	3.0	45
33	Wave packet formulation of the boomerang model for resonant electron-molecule scattering. <i>Journal of Chemical Physics</i> , 1983, 78, 6773-6779.	3.0	116
34	Conversion of bound states to resonances with changing internuclear distance in molecular anions. <i>Journal of Chemical Physics</i> , 1983, 79, 2200-2205.	3.0	38
35	Complex potential-energy function for the 1 ¹ Σ ⁺ shape resonance state of H ₂ ⁻ at the self-consistent-field level. <i>Physical Review A</i> , 1982, 25, 2529-2538.	2.5	55
36	Progress in the application of classical S-matrix theory to inelastic collision processes. <i>Journal of Chemical Physics</i> , 1980, 73, 3191-3197.	3.0	26

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37	Applicability of self-consistent field techniques based on the complex coordinate method to metastable electronic states. Journal of Chemical Physics, 1980, 73, 3268-3273.	3.0	91