David A Micha

List of Publications by Year
in descending order

105	1,735	257450	361022
papers	citations	24 h-index	35 g-index

107	107	107	491
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Relaxation of Photoexcited Electrons at a Nanostructured Si(111) Surface. Journal of Physical Chemistry Letters, 2010, 1, 1073-1077.	4.6	83
2	Time-Dependent Many-Electron Treatment of Electronic Energy and Charge Transfer in Atomic Collisions. Journal of Physical Chemistry A, 1999, 103, 7562-7574.	2.5	63
3	The linearly driven parametric oscillator: Application to collisional energy transfer. Journal of Chemical Physics, 1985, 82, 4926-4936.	3.0	61
4	Compound-State Resonances in Atomâ€"Diatomic-Molecule Collisions. Physical Review, 1967, 162, 88-97.	2.7	52
5	Surface Photovoltage at Nanostructures on Si Surfaces: Ab Initio Results. Journal of Physical Chemistry C, 2009, 113, 3530-3542.	3.1	51
6	Interaction of atoms with solid surfaces: Energy transfer in hyperthermal collisions of Li+ with W(110). Journal of Chemical Physics, 1981, 74, 2054-2058.	3.0	49
7	Variational Methods in the Wave Operator Formalism. A Unified Treatment for Bound and Quasibound Electronic and Molecular States. Journal of Chemical Physics, 1971, 55, 4792-4797.	3.0	46
8	Optical Properties of Doped Silicon Quantum Dots with Crystalline and Amorphous Structures. Journal of Physical Chemistry C, 2011, 115, 19529-19537.	3.1	45
9	Collision Dynamics of Three Interacting Atoms: The Faddeev Equations. Journal of Chemical Physics, 1972, 57, 2184-2192.	3.0	41
10	Variational Methods in the Wave Operator Formalism: Applications in Variationâ€Perturbation Theory and the Theory of Energy Bounds. Journal of Mathematical Physics, 1972, 13, 155-160.	1.1	39
11	Transition operators for atomâ€"atom potentials: The Hilbertâ€"Schmidt expansion. Journal of Chemical Physics, 1978, 68, 4352-4356.	3.0	36
12	Electronically diabatic atomâ€"atom collisions: A selfâ€consistent eikonal approximation. Journal of Chemical Physics, 1992, 97, 1038-1052.	3.0	33
13	Collision dynamics of three interacting atoms: Stripping reactions of Ar++H2and of K+I2. Journal of Chemical Physics, 1976, 64, 1032-1041.	3.0	32
14	Long-lived states in atom-molecule collisions. Accounts of Chemical Research, 1973, 6, 138-144.	15.6	31
15	Modeling the Photovoltage of Doped Si Surfaces. Journal of Physical Chemistry C, 2011, 115, 770-775.	3.1	31
16	Ab initio design of light absorption through silver atomic cluster decoration of TiO₂. Physical Chemistry Chemical Physics, 2018, 20, 19110-19119.	2.8	31
17	Collision dynamics of three interacting atoms: The multipleâ€collision expansion. Journal of Chemical Physics, 1975, 63, 5462-5469.	3.0	30
18	Density matrix theory and calculations of nonlinear yields of CO photodesorbed from Cu(001) by light pulses. Journal of Chemical Physics, 1999, 110, 10562-10575.	3.0	30

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19	Optical Potential for Li-HBr Collisions at Low Energies. Physical Review, 1969, 180, 120-123.	2.7	29
20	Vibrational excitation in collisions between two diatomic molecules using an operator algebra. Journal of Chemical Physics, 1986, 85, 5093-5100.	3.0	29
21	Photoabsorbance and Photovoltage of Crystalline and Amorphous Silicon Slabs with Silver Adsorbates. Journal of Physical Chemistry C, 2012, 116, 25525-25536.	3.1	28
22	Effective Hamiltonian Methods for Molecular Collisions. Advances in Quantum Chemistry, 1974, , 231-287.	0.8	26
23	The Quantumâ€“Classical Density Operator for Electronically Excited Molecular Systems. Advances in Quantum Chemistry, 2004, , 293-314.	0.8	26
24	Electronically diabatic quantum dynamics of molecular desorption. Journal of Chemical Physics, 1995, 103, 3795-3808.	3.0	25
25	Ab initiostudy of the photocurrent at the Au/Si metalâ€“semiconductor nanointerface. Molecular Physics, 2015, 113, 327-335.	1.7	25
26	Atomâ^’polyatomic collisions: The role of pair correlation functions. Journal of Chemical Physics, 1979, 70, 3165-3170.	3.0	24
27	Collision dynamics of three interacting atoms: Permutational symmetry for identical nuclei. Journal of Chemical Physics, 1974, 60, 2480-2487.	3.0	23
28	Atomic modeling of surface photovoltage: Application to Si(1 1 1):H. Chemical Physics Letters, 2008, 461, 266-270.	2.6	23
29	Density matrix theory and computational aspects of quantum dynamics in active medium. International Journal of Quantum Chemistry, 2000, 80, 394-405.	2.0	22
30	Computational Modeling of the Dielectric Function of Silicon Slabs with Varying Thickness. Journal of Physical Chemistry C, 2014, 118, 4429-4436.	3.1	21
31	Direct and indirect electron transfer at a semiconductor surface with an adsorbate: Theory and application to Ag3Si(111):H. Journal of Chemical Physics, 2010, 132, 114702.	3.0	20
32	Collision dynamics of three interacting atoms: Electron transfer in the reactions of K+Br2, BrI, and I2. Journal of Chemical Physics, 1976, 65, 4876-4884.	3.0	19
33	Diatomic transition operators: Results of L2 basis expansions. Journal of Chemical Physics, 1980, 72, 3327-3336.	3.0	19
34	Temporal rearrangement of electronic densities in slow atomic collisions. International Journal of Quantum Chemistry, 1994, 51, 499-518.	2.0	19
35	Optical properties of the Si(111):H surface with adsorbed Ag clusters. International Journal of Quantum Chemistry, 2009, 109, 3694-3704.	2.0	19
36	Equilibrium properties of transitionâ€metal ionâ€“argon clusters via simulated annealing. Journal of Chemical Physics, 1992, 96, 7683-7695.	3.0	18

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37	Density Matrix Treatment of Electronic Rearrangement. Advances in Quantum Chemistry, 1999, , 317-337.	0.8	18
38	Optical properties of amorphous and crystalline silicon surfaces functionalized with Ag_n adsorbates. International Journal of Quantum Chemistry, 2010, 110, 3005-3014.	2.0	18
39	Collision dynamics of three interacting atoms: Energy transfer and dissociation in collinear motions. Journal of Chemical Physics, 1980, 73, 1193-1199.	3.0	17
40	Density matrix treatment of combined instantaneous and delayed dissipation for an electronically excited adsorbate on a solid surface. Journal of Chemical Physics, 2009, 131, 144106.	3.0	17
41	The linearly driven parametric oscillator: Its collisional timeâ€correlation function. Journal of Chemical Physics, 1985, 82, 4937-4942.	3.0	16
42	Density Matrix Treatment of the Nonmarkovian Dissipative Dynamics of Adsorbates on Metal Surfacesâ€. Journal of Physical Chemistry A, 2006, 110, 749-755.	2.5	16
43	Dynamical coupling in the differential equations approach to atom-diatom exchange reactions. Molecular Physics, 1973, 25, 1335-1352.	1.7	15
44	Collision dynamics of three interacting atoms: Vibrationalâ€“rotational excitation in atomâ€“diatom hyperthermal collisions. Journal of Chemical Physics, 1981, 74, 6700-6708.	3.0	15
45	Electronic state representations at molecular potential pseudocrossings. International Journal of Quantum Chemistry, 1982, 22, 971-988.	2.0	15
46	Semiclassical time-correlation function approach to collisional energy transfer into many-atom systems. International Journal of Quantum Chemistry, 1983, 23, 551-560.	2.0	15
47	Anharmonic coupling of vibrational modes in atomâ€“polyatomic collisions: A timeâ€correlation function treatment. Journal of Chemical Physics, 1983, 79, 3794-3806.	3.0	15
48	Photodissociation dynamics from quantumâ€“classical density matrix calculations. Chemical Physics Letters, 2005, 403, 280-286.	2.6	15
49	Density matrix treatment of non-adiabatic photoinduced electron transfer at a semiconductor surface. Journal of Chemical Physics, 2012, 137, 22A521.	3.0	15
50	Calculation of vibrational transition probabilities in molecular collisions: A recursive algebraic procedure. Journal of Chemical Physics, 1989, 91, 924-928.	3.0	14
51	An Eikonal Treatment of Electronically Diabatic Photodissociation:Â Branching Ratios of CH3Iâ€. Journal of Physical Chemistry A, 2001, 105, 2890-2896.	2.5	13
52	Collisional timeâ€correlation functions in the semiclassical limit. III. Application to vibrationalâ€“rotational energy transfer in collisions of Li+with N2. Journal of Chemical Physics, 1987, 86, 760-775.	3.0	12
53	Timeâ€evolution of molecular states in electronically diabatic phenomena. Journal of Chemical Physics, 1992, 97, 8173-8180.	3.0	12
54	From few-atom to many-atom quantum dynamics. Advances in Quantum Chemistry, 2002, 41, 139-159.	0.8	12

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55	Quantum confinement effects on electronic photomobilities at nanostructured semiconductor surfaces: Si(111) without and with adsorbed Ag clusters. Journal of Chemical Physics, 2017, 147, 224703.	3.0	12
56	A computational method for multi-channel scattering calculations. Applications to rotational excitation and long-lived states of He-N2. Chemical Physics Letters, 1974, 28, 341-344.	2.6	11
57	Photodynamics of extended molecular systems. II. Application to the photodissociation of CH3I from vibrationally excited initial states. Journal of Chemical Physics, 1991, 95, 380-390.	3.0	11
58	Angular distributions in electronically adiabatic hyperthermal collisions. An eikonal approach. Journal of Chemical Physics, 1993, 98, 2023-2031.	3.0	11
59	Collision dynamics of three interacting atoms: A method of diatomicsâ€in†molecules. Journal of Chemical Physics, 1977, 66, 1255-1257.	3.0	10
60	Time-evolution of multiconfiguration density functions driven by nuclear motions. International Journal of Quantum Chemistry, 1996, 60, 109-118.	2.0	10
61	Density matrix for non-Markovian dissipative dynamics: A numerical method. Chemical Physics Letters, 2005, 415, 46-50.	2.6	10
62	Interaction potentials and dynamics for Li + F collisions. International Journal of Quantum Chemistry, 1974, 8, 253-262.	2.0	10
63	Generalized Response Theory for a Photoexcited Many-Atom System. Advances in Quantum Chemistry, 2015, 71, 195-220.	0.8	10
64	Model studies of the structure and optical properties of the TiO₂(110) surface with an adsorbed Ag atom. Molecular Physics, 2019, 117, 2267-2274.	1.7	10
65	Collision timeâ€correlation functions in the semiclassical limit. II. Vibrationalâ€“rotational energy transfer in moleculeâ€“molecule collisions. Journal of Chemical Physics, 1987, 86, 750-759.	3.0	9
66	A generalized intermediate picture of quantal time evolution using operator algebraic methods. Application to translationalâ€“vibrational energy transfer in molecular collisions. Journal of Chemical Physics, 1991, 94, 3537-3541.	3.0	9
67	Computational studies of the optical properties of silicon compounds bonding to silver atoms and with group III and V substituents. International Journal of Quantum Chemistry, 2010, 110, 3086-3094.	2.0	9
68	Electronic structure and optical absorbance of doped amorphous silicon slabs. International Journal of Quantum Chemistry, 2012, 112, 300-313.	2.0	9
69	Modeling the surface photovoltage of silicon slabs with varying thickness. Journal of Physics Condensed Matter, 2015, 27, 134204.	1.8	9
70	Optical Models in Molecular Collision Theory. , 1976, , 81-129.		8
71	Longâ€lived states in atomâ€“surface collisions: Reciprocal lattice vector poles. Journal of Chemical Physics, 1980, 73, 6169-6173.	3.0	8
72	Photoinduced electron transfer at a Si(111) nanostructured surface: Effect of varying light wavelength, temperature, and structural parameters. Journal of Chemical Physics, 2013, 138, 184708.	3.0	8

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73	Collisional timeâ€correlation functions for energy transfer: The semiclassical limit. Journal of Chemical Physics, 1986, 84, 3162-3169.	3.0	7
74	Role of Molecular Momentum Distributions in Impulsive Collisions. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1977, 81, 162-164.	0.9	6
75	Collision dynamics of three interacting atoms: The Faddeev equations in a diabatic electronic basis. Journal of Chemical Physics, 1983, 79, 6115-6129.	3.0	6
76	Atomic modeling of structural and optical properties of amorphous silicon. Chemical Physics Letters, 2013, 570, 95-99.	2.6	6
77	Photoconductivities from band states and a dissipative electron dynamics: Si(111) without and with adsorbed Ag clusters. Journal of Chemical Physics, 2016, 144, 024107.	3.0	6
78	Collisional time-correlation functions for molecular interactions. International Journal of Quantum Chemistry, 1986, 30, 773-785.	2.0	5
79	A coupled-channel approach to molecular photodissociation using decay boundary conditions. The Journal of Physical Chemistry, 1991, 95, 8082-8086.	2.9	5
80	Atomic orbital basis sets for molecular interactions. Journal of Computational Chemistry, 1994, 15, 653-661.	3.3	5
81	Molecular photoexcitation in a medium: Density operator approach. International Journal of Quantum Chemistry, 2000, 77, 367-375.	2.0	5
82	Reduced Density Matrix Equations for Combined Instantaneous and Delayed Dissipation in Many-Atom Systems, and their Numerical Treatment. Springer Series in Chemical Physics, 2009, , 363-380.	0.2	5
83	Density matrix calculations of gaseous and adsorbate dynamics in electronically excited molecular systems. International Journal of Quantum Chemistry, 2006, 106, 3371-3382.	2.0	4
84	The Collisional Time-Correlation Function Approach to Molecular Energy Transfer. Advances in Chemical Physics, 2007, , 1-72.	0.3	4
85	Light Absorption by Crystalline and Amorphous Silicon Quantum Dots with Silver Adsorbates and Dopants. Journal of Physical Chemistry C, 2012, 116, 23107-23112.	3.1	4
86	Density Matrix Treatment of Optical Properties in Photovoltaic Materials: Photoconductivity at a Semiconductor Surface. ACS Symposium Series, 2015, , 151-167.	0.5	4
87	Recent developments in the theory of reactive molecular collisions. International Journal of Quantum Chemistry, 1974, 8, 263-269.	2.0	3
88	Electronic Relaxation of Photoexcited Open and Closed Shell Adsorbates on Semiconductors: Ag and Ag2 on TiO2. Journal of Chemical Physics, 2022, 156, 104705.	3.0	3
89	Atom-Diatom Resonances Within a Many-Body Approach to Reactive Scattering. ACS Symposium Series, 1984, , 401-419.	0.5	2
90	Variationally improved transition amplitudes from time-dependent Hartree-Fock wave functions: Application to He + He2+ collisions. International Journal of Quantum Chemistry, 1986, 30, 689-697.	2.0	2

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91	Construction of effective Hamiltonians for timeâ€dependent phenomena from variational principles. Journal of Chemical Physics, 1991, 95, 3607-3613.	3.0	2
92	Operator formalisms of reactive molecular scattering. International Journal of Quantum Chemistry, 1976, 10, 259-266.	2.0	2
93	Self-Consistent coupling of atomic orbitals to a moving charge. International Journal of Quantum Chemistry, 1994, 52, 49-64.	2.0	1
94	A study of single-electron and total energies for some pairs of noble gas atoms. International Journal of Quantum Chemistry, 1974, 8, 229-240.	2.0	1
95	Time-dependent many-electron phenomena in quantum molecular dynamics. Molecular Physics, 2010, 108, 3213-3222.	1.7	1
96	Time-dependent methods of quantum dynamics: from few atoms to condensed matter. Molecular Physics, 2010, 108, 2877-2890.	1.7	1
97	Quantum Partitioning Methods for Few-Atom and Many-Atom Dynamics. Advances in Quantum Chemistry, 2017, 74, 107-128.	0.8	1
98	Optical Properties of the TiO₂(110) Surface with Adsorbed Ag Atoms Relevant to Photocatalysis and Photovoltaics. ACS Symposium Series, 2019, , 47-66.	0.5	1
99	Multichannel treatment of penning ionization in He* (1s2s, 3S) + ar with discretization of the electronic continuum. International Journal of Quantum Chemistry, 2009, 16, 569-577.	2.0	0
100	Cumulant expansion of time-correlation functions for collisional energy transfer. International Journal of Quantum Chemistry, 2009, 20, 643-652.	2.0	0
101	Time-correlation function approach to molecular anharmonicity in hyperthermal atom-molecule collisions. International Journal of Quantum Chemistry, 1981, 20, 653-661.	2.0	0
102	A self-consistent eikonal treatment of photodissociation by visible radiation. International Journal of Quantum Chemistry, 2009, 22, 377-390.	2.0	0
103	Molecular photodissociation by visible and ultraviolet radiation: Time evolution and state-to-state cross sections. International Journal of Quantum Chemistry, 2009, 24, 192-192.	2.0	0
104	Collisional time-correlation functions for molecular interactions. International Journal of Quantum Chemistry, 2009, 28, 443-455.	2.0	0
105	Chemical reactions in the gas phase and in condensed matter: From wavefunctions to density operators. International Journal of Quantum Chemistry, 2009, 109, 2937-2942.	2.0	0