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	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
2	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
3	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
4	Ab initio design of light absorption through silver atomic cluster decoration of TiO₂. Physical Chemistry Chemical Physics, 2018, 20, 19110-19119.	2.8	31
5	Quantum Partitioning Methods for Few-Atom and Many-Atom Dynamics. Advances in Quantum Chemistry, 2017, 74, 107-128.	0.8	1
6	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
7	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
8	Density Matrix Treatment of Optical Properties in Photovoltaic Materials: Photoconductivity at a Semiconductor Surface. ACS Symposium Series, 2015, , 151-167.	0.5	4
9	Generalized Response Theory for a Photoexcited Many-Atom System. Advances in Quantum Chemistry, 2015, 71, 195-220.	0.8	10
10	Modeling the surface photovoltage of silicon slabs with varying thickness. Journal of Physics Condensed Matter, 2015, 27, 134204.	1.8	9
11	Ab initiostudy of the photocurrent at the Au/Si metalâ€“semiconductor nanointerface. Molecular Physics, 2015, 113, 327-335.	1.7	25
12	Computational Modeling of the Dielectric Function of Silicon Slabs with Varying Thickness. Journal of Physical Chemistry C, 2014, 118, 4429-4436.	3.1	21
13	Atomic modeling of structural and optical properties of amorphous silicon. Chemical Physics Letters, 2013, 570, 95-99.	2.6	6
14	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
15	Density matrix treatment of non-adiabatic photoinduced electron transfer at a semiconductor surface. Journal of Chemical Physics, 2012, 137, 22A521.	3.0	15
16	Photoabsorbance and Photovoltage of Crystalline and Amorphous Silicon Slabs with Silver Adsorbates. Journal of Physical Chemistry C, 2012, 116, 25525-25536.	3.1	28
17	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
18	Electronic structure and optical absorbance of doped amorphous silicon slabs. International Journal of Quantum Chemistry, 2012, 112, 300-313.	2.0	9

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19	Modeling the Photovoltage of Doped Si Surfaces. Journal of Physical Chemistry C, 2011, 115, 770-775.	3.1	31
20	Optical Properties of Doped Silicon Quantum Dots with Crystalline and Amorphous Structures. Journal of Physical Chemistry C, 2011, 115, 19529-19537.	3.1	45
21	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
22	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
23	Relaxation of Photoexcited Electrons at a Nanostructured Si(111) Surface. Journal of Physical Chemistry Letters, 2010, 1, 1073-1077.	4.6	83
24	Time-dependent many-electron phenomena in quantum molecular dynamics. Molecular Physics, 2010, 108, 3213-3222.	1.7	1
25	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
26	Time-dependent methods of quantum dynamics: from few atoms to condensed matter. Molecular Physics, 2010, 108, 2877-2890.	1.7	1
27	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
28	Cumulant expansion of time-correlation functions for collisional energy transfer. International Journal of Quantum Chemistry, 2009, 20, 643-652.	2.0	0
29	A self-consistent eikonal treatment of photodissociation by visible radiation. International Journal of Quantum Chemistry, 2009, 22, 377-390.	2.0	0
30	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
31	Collisional time-correlation functions for molecular interactions. International Journal of Quantum Chemistry, 2009, 28, 443-455.	2.0	0
32	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
33	Optical properties of the Si(111):H surface with adsorbed Ag clusters. International Journal of Quantum Chemistry, 2009, 109, 3694-3704.	2.0	19
34	Surface Photovoltage at Nanostructures on Si Surfaces: Ab Initio Results. Journal of Physical Chemistry C, 2009, 113, 3530-3542.	3.1	51
35	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
36	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

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37	Atomic modeling of surface photovoltage: Application to Si(1 1 1):H. Chemical Physics Letters, 2008, 461, 266-270.	2.6	23
38	The Collisional Time-Correlation Function Approach to Molecular Energy Transfer. Advances in Chemical Physics, 2007, , 1-72.	0.3	4
39	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
40	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
41	Photodissociation dynamics from quantumâ€“classical density matrix calculations. Chemical Physics Letters, 2005, 403, 280-286.	2.6	15
42	Density matrix for non-Markovian dissipative dynamics: A numerical method. Chemical Physics Letters, 2005, 415, 46-50.	2.6	10
43	The Quantumâ€“Classical Density Operator for Electronically Excited Molecular Systems. Advances in Quantum Chemistry, 2004, , 293-314.	0.8	26
44	From few-atom to many-atom quantum dynamics. Advances in Quantum Chemistry, 2002, 41, 139-159.	0.8	12
45	An Eikonal Treatment of Electronically Diabatic Photodissociation:Â Branching Ratios of CH3Iâ€. Journal of Physical Chemistry A, 2001, 105, 2890-2896.	2.5	13
46	Molecular photoexcitation in a medium: Density operator approach. International Journal of Quantum Chemistry, 2000, 77, 367-375.	2.0	5
47	Density matrix theory and computational aspects of quantum dynamics in active medium. International Journal of Quantum Chemistry, 2000, 80, 394-405.	2.0	22
48	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
49	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
50	Density Matrix Treatment of Electronic Rearrangement. Advances in Quantum Chemistry, 1999, , 317-337.	0.8	18
51	Time-evolution of multiconfiguration density functions driven by nuclear motions. International Journal of Quantum Chemistry, 1996, 60, 109-118.	2.0	10
52	Electronically diabatic quantum dynamics of molecular desorption. Journal of Chemical Physics, 1995, 103, 3795-3808.	3.0	25
53	Temporal rearrangement of electronic densities in slow atomic collisions. International Journal of Quantum Chemistry, 1994, 51, 499-518.	2.0	19
54	Self-Consistent coupling of atomic orbitals to a moving charge. International Journal of Quantum Chemistry, 1994, 52, 49-64.	2.0	1

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55	Atomic orbital basis sets for molecular interactions. Journal of Computational Chemistry, 1994, 15, 653-661.	3.3	5
56	Angular distributions in electronically adiabatic hyperthermal collisions. An eikonal approach. Journal of Chemical Physics, 1993, 98, 2023-2031.	3.0	11
57	Electronically diabatic atomâ€“atom collisions: A selfâ€consistent eikonal approximation. Journal of Chemical Physics, 1992, 97, 1038-1052.	3.0	33
58	Equilibrium properties of transitionâ€metal ionâ€“argon clusters via simulated annealing. Journal of Chemical Physics, 1992, 96, 7683-7695.	3.0	18
59	Timeâ€evolution of molecular states in electronically diabatic phenomena. Journal of Chemical Physics, 1992, 97, 8173-8180.	3.0	12
60	A coupled-channel approach to molecular photodissociation using decay boundary conditions. The Journal of Physical Chemistry, 1991, 95, 8082-8086.	2.9	5
61	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
62	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
63	Construction of effective Hamiltonians for timeâ€dependent phenomena from variational principles. Journal of Chemical Physics, 1991, 95, 3607-3613.	3.0	2
64	Calculation of vibrational transition probabilities in molecular collisions: A recursive algebraic procedure. Journal of Chemical Physics, 1989, 91, 924-928.	3.0	14
65	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
66	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
67	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
68	Collisional time-correlation functions for molecular interactions. International Journal of Quantum Chemistry, 1986, 30, 773-785.	2.0	5
69	Collisional timeâ€correlation functions for energy transfer: The semiclassical limit. Journal of Chemical Physics, 1986, 84, 3162-3169.	3.0	7
70	Vibrational excitation in collisions between two diatomic molecules using an operator algebra. Journal of Chemical Physics, 1986, 85, 5093-5100.	3.0	29
71	The linearly driven parametric oscillator: Its collisional timeâ€correlation function. Journal of Chemical Physics, 1985, 82, 4937-4942.	3.0	16
72	The linearly driven parametric oscillator: Application to collisional energy transfer. Journal of Chemical Physics, 1985, 82, 4926-4936.	3.0	61

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73	Atom-Diatom Resonances Within a Many-Body Approach to Reactive Scattering. ACS Symposium Series, 1984, , 401-419.	0.5	2
74	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
75	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
76	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
77	Electronic state representations at molecular potential pseudocrossings. International Journal of Quantum Chemistry, 1982, 22, 971-988.	2.0	15
78	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
79	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
80	Time-correlation function approach to molecular anharmonicity in hyperthermal atom-molecule collisions. International Journal of Quantum Chemistry, 1981, 20, 653-661.	2.0	0
81	Longâ€lived states in atomâ€“surface collisions: Reciprocal lattice vector poles. Journal of Chemical Physics, 1980, 73, 6169-6173.	3.0	8
82	Diatomic transition operators: Results of L2 basis expansions. Journal of Chemical Physics, 1980, 72, 3327-3336.	3.0	19
83	Collision dynamics of three interacting atoms: Energy transfer and dissociation in collinear motions. Journal of Chemical Physics, 1980, 73, 1193-1199.	3.0	17
84	Atomâ”polyatomic collisions: The role of pair correlation functions. Journal of Chemical Physics, 1979, 70, 3165-3170.	3.0	24
85	Transition operators for atomâ€“atom potentials: The Hilbertâ€“Schmidt expansion. Journal of Chemical Physics, 1978, 68, 4352-4356.	3.0	36
86	Collision dynamics of three interacting atoms: A method of diatomicsâ€inâ€molecules. Journal of Chemical Physics, 1977, 66, 1255-1257.	3.0	10
87	Role of Molecular Momentum Distributions in Impulsive Collisions. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1977, 81, 162-164.	0.9	6
88	Optical Models in Molecular Collision Theory. , 1976, , 81-129.		8
89	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
90	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

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91	Operator formalisms of reactive molecular scattering. International Journal of Quantum Chemistry, 1976, 10, 259-266.	2.0	2
92	Collision dynamics of three interacting atoms: The multipleâ€collision expansion. Journal of Chemical Physics, 1975, 63, 5462-5469.	3.0	30
93	Collision dynamics of three interacting atoms: Permutational symmetry for identical nuclei. Journal of Chemical Physics, 1974, 60, 2480-2487.	3.0	23
94	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
95	Effective Hamiltonian Methods for Molecular Collisions. Advances in Quantum Chemistry, 1974, , 231-287.	0.8	26
96	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
97	Interaction potentials and dynamics for Li + F collisions. International Journal of Quantum Chemistry, 1974, 8, 253-262.	2.0	10
98	Recent developments in the theory of reactive molecular collisions. International Journal of Quantum Chemistry, 1974, 8, 263-269.	2.0	3
99	Long-lived states in atom-molecule collisions. Accounts of Chemical Research, 1973, 6, 138-144.	15.6	31
100	Dynamical coupling in the differential equations approach to atom-diatom exchange reactions. Molecular Physics, 1973, 25, 1335-1352.	1.7	15
101	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
102	Collision Dynamics of Three Interacting Atoms: The Faddeev Equations. Journal of Chemical Physics, 1972, 57, 2184-2192.	3.0	41
103	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
104	Optical Potential for Li-HBr Collisions at Low Energies. Physical Review, 1969, 180, 120-123.	2.7	29
105	Compound-State Resonances in Atomâ€”Diatomic-Molecule Collisions. Physical Review, 1967, 162, 88-97.	2.7	52