

Abraham Nitzan

List of Publications by Year in descending order

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152
papers

18,105
citations

22099

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130
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154
all docs

154
docs citations

154
times ranked

11003
citing authors

#	ARTICLE	IF	CITATIONS
1	Electron Transport in Molecular Wire Junctions. <i>Science</i> , 2003, 300, 1384-1389.	6.0	2,173
2	Electromagnetic theory of enhanced Raman scattering by molecules adsorbed on rough surfaces. <i>Journal of Chemical Physics</i> , 1980, 73, 3023-3037.	1.2	1,009
3	Chemical Dynamics in Condensed Phases. , 2006, , .		908
4	ELECTRON TRANSMISSION THROUGH MOLECULES AND MOLECULAR INTERFACES. <i>Annual Review of Physical Chemistry</i> , 2001, 52, 681-750.	4.8	874
5	Covalently bonded single-molecule junctions with stable and reversible photoswitched conductivity. <i>Science</i> , 2016, 352, 1443-1445.	6.0	697
6	Spectroscopic properties of molecules interacting with small dielectric particles. <i>Journal of Chemical Physics</i> , 1981, 75, 1139-1152.	1.2	676
7	Molecular transport junctions: vibrational effects. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 103201.	0.7	618
8	The enhancement of Raman scattering, resonance Raman scattering, and fluorescence from molecules adsorbed on a rough silver surface. <i>Journal of Chemical Physics</i> , 1983, 78, 5324-5338.	1.2	465
9	Thermal conductance through molecular wires. <i>Journal of Chemical Physics</i> , 2003, 119, 6840-6855.	1.2	338
10	Spin-Boson Thermal Rectifier. <i>Physical Review Letters</i> , 2005, 94, 034301.	2.9	334
11	Concepts in the design and engineering of single-molecule electronic devices. <i>Nature Reviews Physics</i> , 2019, 1, 211-230.	11.9	327
12	Inelastic electron tunneling spectroscopy in molecular junctions: Peaks and dips. <i>Journal of Chemical Physics</i> , 2004, 121, 11965-11979.	1.2	320
13	The interaction between electromagnetic resonances and its role in spectroscopic studies of molecules adsorbed on colloidal particles or metal spheres. <i>Surface Science</i> , 1981, 110, 189-204.	0.8	303
14	Electron Transfer Rates in Bridged Molecular Systems 2. A Steady-State Analysis of Coherent Tunneling and Thermal Transitions. <i>Journal of Physical Chemistry B</i> , 2000, 104, 3817-3829.	1.2	298
15	Hysteresis, Switching, and Negative Differential Resistance in Molecular Junctions: A Polaron Model. <i>Nano Letters</i> , 2005, 5, 125-130.	4.5	296
16	Dynamic bond percolation theory: A microscopic model for diffusion in dynamically disordered systems. I. Definition and one-dimensional case. <i>Journal of Chemical Physics</i> , 1983, 79, 3133-3142.	1.2	279
17	Nuclear Coupling and Polarization in Molecular Transport Junctions: Beyond Tunneling to Function. <i>Science</i> , 2008, 319, 1056-1060.	6.0	273
18	Theoretical model for enhanced photochemistry on rough surfaces. <i>Journal of Chemical Physics</i> , 1981, 75, 2205-2214.	1.2	254

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19	A Lattice Relaxation Algorithm for Three-Dimensional Poisson-Nernst-Planck Theory with Application to Ion Transport through the Gramicidin A Channel. <i>Biophysical Journal</i> , 1999, 76, 642-656.	0.2	254
20	Photoconductance and inverse photoconductance in films of functionalized metal nanoparticles. <i>Nature</i> , 2009, 460, 371-375.	13.7	239
21	Energy gap law for vibrational relaxation of a molecule in a dense medium. <i>Journal of Chemical Physics</i> , 1975, 63, 200-207.	1.2	221
22	Some features of vibrational relaxation of a diatomic molecule in a dense medium. <i>Journal of Chemical Physics</i> , 1974, 60, 3929-3934.	1.2	219
23	Resonant inelastic tunneling in molecular junctions. <i>Physical Review B</i> , 2006, 73, .	1.1	204
24	A Relationship between Electron-Transfer Rates and Molecular Conduction. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2677-2679.	1.1	188
25	Vibrational relaxation of a molecule in a dense medium. <i>Molecular Physics</i> , 1973, 25, 713-734.	0.8	187
26	Heat conduction in molecular transport junctions. <i>Physical Review B</i> , 2007, 75, .	1.1	187
27	Electron Transfer Rates in Bridged Molecular Systems: A Phenomenological Approach to Relaxation. <i>Journal of Physical Chemistry A</i> , 1997, 101, 6158-6164.	1.1	182
28	Photophysics and photochemistry near surfaces and small particles. <i>Surface Science</i> , 1985, 158, 165-189.	0.8	177
29	Molecular optoelectronics: the interaction of molecular conduction junctions with light. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 9421.	1.3	156
30	On the ionization potential of small metal and dielectric particles. <i>Journal of Chemical Physics</i> , 1988, 88, 5076-5085.	1.2	149
31	Molecular Wires Acting as Coherent Quantum Ratchets. <i>Physical Review Letters</i> , 2002, 88, 228305.	2.9	144
32	Local fields in cavity sites of rough dielectric surfaces. <i>Chemical Physics Letters</i> , 1984, 111, 449-454.	1.2	135
33	A rate constant expression for charge transfer through fluctuating bridges. <i>Journal of Chemical Physics</i> , 2003, 119, 5782-5788.	1.2	133
34	Accelerated energy transfer between molecules near a solid particle. <i>Chemical Physics Letters</i> , 1984, 104, 31-37.	1.2	130
35	Molecular rectification: why is it so rare?. <i>Chemical Physics</i> , 2002, 281, 147-150.	0.9	128
36	Vibronic effects in off-resonant molecular wire conduction. <i>Journal of Chemical Physics</i> , 2003, 118, 6072-6082.	1.2	122

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37	Current-induced nonequilibrium vibrations in single-molecule devices. <i>Physical Review B</i> , 2006, 73, .	1.1	119
38	On the Line Widths of Vibrational Features in Inelastic Electron Tunneling Spectroscopy. <i>Nano Letters</i> , 2004, 4, 1605-1611.	4.5	113
39	The Role of the Dielectric Barrier in Narrow Biological Channels: A Novel Composite Approach to Modeling Single-Channel Currents. <i>Biophysical Journal</i> , 2003, 84, 3646-3661.	0.2	111
40	Nonlinear Charge Transport in Redox Molecular Junctions: A Marcus Perspective. <i>ACS Nano</i> , 2011, 5, 6669-6685.	7.3	111
41	Heating in current carrying molecular junctions. <i>Journal of Chemical Physics</i> , 2002, 117, 3915-3927.	1.2	99
42	Heat rectification in molecular junctions. <i>Journal of Chemical Physics</i> , 2005, 122, 194704.	1.2	99
43	Can photochemistry be enhanced on rough surfaces?. <i>Journal of Chemical Physics</i> , 1981, 74, 5321-5322.	1.2	98
44	Activated Conduction in Microscopic Molecular Junctions. <i>Journal of Physical Chemistry B</i> , 2000, 104, 2790-2793.	1.2	96
45	Comparison of Dynamic Lattice Monte Carlo Simulations and the Dielectric Self-Energy Poisson-Nernst-Planck Continuum Theory for Model Ion Channels. <i>Journal of Physical Chemistry B</i> , 2004, 108, 2006-2015.	1.2	93
46	Tunneling Time for Electron Transfer Reactions. <i>Journal of Physical Chemistry B</i> , 2000, 104, 5661-5665.	1.2	92
47	Optical properties of current carrying molecular wires. <i>Journal of Chemical Physics</i> , 2006, 124, 234709.	1.2	91
48	Inelastic tunneling effects on noise properties of molecular junctions. <i>Physical Review B</i> , 2006, 74, .	1.1	89
49	A Dynamic Lattice Monte Carlo Model of Ion Transport in Inhomogeneous Dielectric Environments: A Method and Implementation. <i>Journal of Physical Chemistry B</i> , 2000, 104, 12324-12338.	1.2	86
50	Cooling mechanisms in molecular conduction junctions. <i>Physical Review B</i> , 2009, 80, .	1.1	85
51	Rectification of laser-induced electronic transport through molecules. <i>Journal of Chemical Physics</i> , 2003, 118, 3283-3293.	1.2	81
52	Circular Currents in Molecular Wires. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20583-20594.	1.5	77
53	Stochastic classical trajectory approach to relaxation phenomena. I. Vibrational relaxation of impurity molecules in solid matrices. <i>Journal of Chemical Physics</i> , 1978, 69, 336.	1.2	75
54	Inelastic effects in molecular junction transport: scattering and self-consistent calculations for the Seebeck coefficient. <i>Molecular Physics</i> , 2008, 106, 397-404.	0.8	74

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55	Optics of exciton-plasmon nanomaterials. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 443003.	0.7	73
56	Multiconfiguration time-dependent self-consistent field approximations in the numerical solution of quantum dynamical problems. <i>Computer Physics Communications</i> , 1991, 63, 243-258.	3.0	70
57	Numerical studies of the interaction of an atomic sample with the electromagnetic field in two dimensions. <i>Physical Review A</i> , 2011, 84, .	1.0	68
58	Raman scattering in current-carrying molecular junctions. <i>Journal of Chemical Physics</i> , 2009, 130, 144109.	1.2	66
59	Irreversibility and Hysteresis in Redox Molecular Conduction Junctions. <i>Journal of the American Chemical Society</i> , 2013, 135, 9420-9432.	6.6	62
60	Conduction in molecular junctions: inelastic effects. <i>Chemical Physics</i> , 2002, 281, 235-256.	0.9	61
61	Inelastic transport in the Coulomb blockade regime within a nonequilibrium atomic limit. <i>Physical Review B</i> , 2008, 78, .	1.1	59
62	On the relationship between molecular state and single electron pictures in simple electrochemical junctions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 13746.	1.3	59
63	Asymmetric electron transmission across asymmetric alkanethiol bilayer junctions. <i>Journal of Electroanalytical Chemistry</i> , 2003, 550-551, 337-350.	1.9	57
64	Steady-state quantum mechanics of thermally relaxing systems. <i>Chemical Physics</i> , 2001, 268, 315-335.	0.9	56
65	Electron transfer in confined electromagnetic fields. <i>Journal of Chemical Physics</i> , 2019, 150, 174122.	1.2	56
66	Theoretical studies of the spectroscopy of excess electrons in water clusters. <i>Journal of Chemical Physics</i> , 1990, 93, 6226-6238.	1.2	55
67	Molecular Wire Junctions: Tuning the Conductance. <i>Journal of Physical Chemistry B</i> , 2003, 107, 91-95.	1.2	55
68	Computing vibrational energy relaxation for high-frequency modes in condensed environments. <i>Journal of Chemical Physics</i> , 1997, 107, 10470-10479.	1.2	54
69	On the electrostatic potential profile in biased molecular wires. <i>Journal of Chemical Physics</i> , 2002, 117, 10837-10841.	1.2	54
70	Molecular Transport Junctions: Current from Electronic Excitations in the Leads. <i>Physical Review Letters</i> , 2006, 96, 166803.	2.9	54
71	The relationship between electron transfer rate and molecular conduction 2. The sequential hopping case. <i>Israel Journal of Chemistry</i> , 2002, 42, 163-166.	1.0	53
72	Molecules Take the Heat. <i>Science</i> , 2007, 317, 759-760.	6.0	51

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73	Electron transfer across a thermal gradient. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 9421-9429.	3.3	50
74	Electron tunneling through water layers: Effect of layer structure and thickness. Journal of Chemical Physics, 1997, 106, 6647-6654.	1.2	49
75	Transport in State Space: Voltage-Dependent Conductance Calculations of Benzene-1,4-dithiol. Nano Letters, 2009, 9, 1770-1774.	4.5	49
76	Label-Free Dynamic Detection of Single-Molecule Nucleophilic-Substitution Reactions. Nano Letters, 2018, 18, 4156-4162.	4.5	48
77	Surface hopping with a manifold of electronic states. II. Application to the many-body Anderson-Holstein model. Journal of Chemical Physics, 2015, 142, 084110.	1.2	46
78	Molecular Transport Junctions: Asymmetry in Inelastic Tunneling Processes. Journal of Physical Chemistry B, 2005, 109, 8519-8522.	1.2	43
79	Raman Scattering from Nonequilibrium Molecular Conduction Junctions. Nano Letters, 2009, 9, 758-762.	4.5	43
80	Transient resonance structures in electron tunneling through water. Journal of Chemical Physics, 1999, 111, 7558-7566.	1.2	42
81	The electrostatic potential profile along a biased molecular wire: A model quantum-mechanical calculation. Journal of Chemical Physics, 2003, 118, 3756-3763.	1.2	42
82	Numerical computation of tunneling fluxes. Journal of Chemical Physics, 2002, 117, 10817-10826.	1.2	41
83	The non-linear response of molecular junctions: the polaron model revisited. Journal of Physics Condensed Matter, 2008, 20, 374107.	0.7	39
84	Surface hopping with a manifold of electronic states. III. Transients, broadening, and the Marcus picture. Journal of Chemical Physics, 2015, 142, 234106.	1.2	38
85	Solvation effects on molecular pure radiative lifetime and absorption oscillator strength in clusters. Journal of Chemical Physics, 1990, 93, 147-158.	1.2	36
86	NEGF-HF Method in Molecular Junction Property Calculations. Annals of the New York Academy of Sciences, 2003, 1006, 48-67.	1.8	35
87	Electron transfer mechanism and the locality of the system-bath interaction: A comparison of local, semilocal, and pure dephasing models. Journal of Chemical Physics, 2006, 124, 074501.	1.2	35
88	Charge-carrier-induced frequency renormalization, damping, and heating of vibrational modes in nanoscale junctions. Physical Review B, 2013, 88, .	1.1	35
89	Effects of vibrational relaxation on molecular electronic transitions. Journal of Chemical Physics, 1973, 58, 2412-2434.	1.2	33
90	Effects of initial state preparation on the distance dependence of electron transfer through molecular bridges and wires. Journal of Chemical Physics, 2003, 119, 6271-6276.	1.2	33

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91	Correlated dynamic percolation: Many bond effective-medium theory. <i>Journal of Chemical Physics</i> , 1989, 90, 3784-3794.	1.2	32
92	Raman scattering from biased molecular conduction junctions: The electronic background and its temperature. <i>Physical Review B</i> , 2011, 84, .	1.1	32
93	Electromagnetic Theory: A Spheroidal Model. , 1982, , 89-107.		32
94	Compensation of Coulomb Blocking and Energy Transfer in the Current Voltage Characteristic of Molecular Conduction Junctions. <i>Nano Letters</i> , 2012, 12, 2228-2232.	4.5	31
95	Electron transfer at thermally heterogeneous molecule-metal interfaces. <i>Journal of Chemical Physics</i> , 2017, 146, .	1.2	31
96	Electron-Transfer-Induced Thermal and Thermoelectric Rectification. <i>Physical Review Letters</i> , 2018, 121, 247704.	2.9	31
97	Dynamic percolation theory for diffusion of interacting particles. <i>Journal of Chemical Physics</i> , 1990, 92, 1329-1338.	1.2	28
98	Dynamically disordered hopping, glass transition, and polymer electrolytes. <i>Journal of Chemical Physics</i> , 1995, 103, 3253-3261.	1.2	27
99	Nuclear Dynamics at Molecule-Metal Interfaces: A Pseudoparticle Perspective. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 4898-4903.	2.1	27
100	Raman scattering from molecular conduction junctions: Charge transfer mechanism. <i>Physical Review B</i> , 2012, 85, .	1.1	26
101	Electron Tunneling through Water Layers: Effect of Polarizability. <i>Journal of Physical Chemistry A</i> , 1997, 101, 429-433.	1.1	25
102	Numerical Simulations of Electron Tunneling Currents in Water. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10790-10796.	1.1	25
103	Primary events following electron injection into water and adsorbed water layers. <i>Journal of Chemical Physics</i> , 1990, 93, 6535-6542.	1.2	24
104	Radiative properties of solvated molecules in dielectric clusters and small particles. <i>Journal of Chemical Physics</i> , 1991, 95, 686-699.	1.2	24
105	Numerical simulations of electron tunneling in water. <i>Journal of Chemical Physics</i> , 1996, 104, 1549-1559.	1.2	24
106	Electron Transmission through Molecular Layers: Numerical Simulations and Theoretical Considerations. <i>Accounts of Chemical Research</i> , 1999, 32, 854-861.	7.6	24
107	Electrothermal Transistor Effect and Cyclic Electronic Currents in Multithermal Charge Transfer Networks. <i>Physical Review Letters</i> , 2017, 118, 207201.	2.9	24
108	Coherent charge transport through molecular wires: Exciton blocking and current from electronic excitations in the wire. <i>Physical Review B</i> , 2010, 81, .	1.1	23

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109	Numerical Calculations of Radiative and Non-Radiative Relaxation of Molecules Near Metal Particles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 10545-10551.	1.5	22
110	The effect of small cluster environment on molecular oscillator strengths and spectra. <i>Journal of Chemical Physics</i> , 1988, 88, 3516-3523.	1.2	21
111	Perturbation theory approach to tunneling: Direct and resonance transmission in super-exchange models. <i>Journal of Chemical Physics</i> , 1999, 111, 1569-1579.	1.2	21
112	Polaron formation: Ehrenfest dynamics vs. exact results. <i>Journal of Chemical Physics</i> , 2013, 138, 044112.	1.2	21
113	Wiedemann-Franz Law for Molecular Hopping Transport. <i>Nano Letters</i> , 2020, 20, 989-993.	4.5	21
114	Asymmetric tunneling through ordered molecular layers. <i>Journal of Chemical Physics</i> , 1997, 106, 1291-1293.	1.2	20
115	Nonlinear hopping transport in ring systems and open channels. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 645-654.	1.3	20
116	Dielectric environment effects on surface-enhanced resonant electromagnetic processes. <i>The Journal of Physical Chemistry</i> , 1982, 86, 2011-2015.	2.9	19
117	A treatment of vibrational relaxation without the rotating wave approximation. <i>Chemical Physics</i> , 1976, 16, 49-59.	0.9	18
118	Radiative and nonradiative decay rates of molecules adsorbed on clusters of small dielectric particles. <i>Journal of Chemical Physics</i> , 1985, 82, 3831-3840.	1.2	18
119	Unidirectional hopping transport of interacting particles on a finite chain. <i>Journal of Chemical Physics</i> , 2010, 133, 054102.	1.2	18
120	Electron-transfer-induced and phononic heat transport in molecular environments. <i>Journal of Chemical Physics</i> , 2017, 147, 124101.	1.2	18
121	Averaged local field intensities in composite materials. <i>Chemical Physics Letters</i> , 1982, 88, 409-412.	1.2	16
122	Traversal time for electron tunneling in water. <i>Journal of Chemical Physics</i> , 2001, 114, 9205-9208.	1.2	16
123	Molecular electronic states near metal surfaces at equilibrium using potential of mean force and numerical renormalization group methods: Hysteresis revisited. <i>Journal of Chemical Physics</i> , 2016, 144, 074109.	1.2	15
124	Quantum transport with two interacting conduction channels. <i>Journal of Chemical Physics</i> , 2013, 138, 174111.	1.2	14
125	Quadratic effects in multiphonon transition rates in solids. <i>Chemical Physics</i> , 1977, 26, 413-419.	0.9	13
126	Inelastic effects in electron tunneling through water layers. <i>Journal of Chemical Physics</i> , 2001, 115, 2681-2694.	1.2	13

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127	Tight-Binding Description of the STM Image of Molecular Chains. Israel Journal of Chemistry, 2004, 44, 133-143.	1.0	13
128	Irreversibility in redox molecular conduction: single versus double metal-molecule interfaces. Electrochimica Acta, 2015, 160, 363-375.	2.6	13
129	Evaluation of dynamical properties of open quantum systems using the driven Liouville-von Neumann approach: methodological considerations. Molecular Physics, 2019, 117, 2083-2096.	0.8	13
130	Heat conduction in polymer chains with controlled end-to-end distance. Journal of Chemical Physics, 2020, 153, 164903.	1.2	13
131	Phenomenology of resonance Raman scattering and resonance fluorescence from thermally relaxing systems. Chemical Physics, 1979, 41, 163-181.	0.9	12
132	Random walk in dynamically disordered systems. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1987, 56, 853-859.	0.6	12
133	Cooperative Effects in Inelastic Tunneling. Journal of Physical Chemistry B, 2013, 117, 4449-4453.	1.2	12
134	Ehrenfest+R dynamics. II. A semiclassical QED framework for Raman scattering. Journal of Chemical Physics, 2019, 150, 044103.	1.2	12
135	Dynamic bond percolation theory for diffusion of interacting particles: Tracer diffusion in a binary mixture lattice gas. Journal of Chemical Physics, 1990, 93, 5918-5934.	1.2	11
136	Stochastic simulation of nonequilibrium heat conduction in extended molecular junctions. Journal of Chemical Physics, 2020, 153, 144113.	1.2	11
137	Local Atomic Heat Currents and Classical Interference in Single-Molecule Heat Conduction. Journal of Physical Chemistry Letters, 2020, 11, 4261-4268.	2.1	11
138	Tracer diffusion of interacting particles on incomplete lattices: Effective medium approximation. Journal of Chemical Physics, 1990, 93, 3420-3426.	1.2	10
139	Energy, Work, Entropy, and Heat Balance in Marcus Molecular Junctions. Journal of Physical Chemistry B, 2020, 124, 2632-2642.	1.2	10
140	Electron tunneling through a dielectric barrier. Journal of Chemical Physics, 1994, 101, 8224-8237.	1.2	8
141	Energy transfer and thermoelectricity in molecular junctions in non-equilibrated solvents. Journal of Chemical Physics, 2022, 156, 094306.	1.2	8
142	Foundations of Molecular Electronics – Charge Transport in Molecular Conduction Junctions. , 2006, , 13-54.		7
143	Transport and thermodynamics in quantum junctions: A scattering approach. Journal of Chemical Physics, 2020, 152, 244126.	1.2	5
144	Averaged local field intensities in composite films. Surface Science, 1983, 130, 124-154.	0.8	4

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145	Upside/Downside statistical mechanics of nonequilibrium Brownian motion. I. Distributions, moments, and correlation functions of a free particle. <i>Journal of Chemical Physics</i> , 2018, 148, 044101.	1.2	4
146	Coupling, lifetimes, and strong coupling maps for single molecules at plasmonic interfaces. <i>Journal of Chemical Physics</i> , 2022, 156, 154303.	1.2	4
147	Mechanical properties of dynamically disordered networks. <i>Journal of Non-Crystalline Solids</i> , 1991, 131-133, 1018-1021.	1.5	3
148	On the widths of Stokes lines in Raman scattering from molecules adsorbed at metal surfaces and in molecular conduction junctions. <i>Journal of Chemical Physics</i> , 2016, 144, 244114.	1.2	3
149	Upside/Downside statistical mechanics of nonequilibrium Brownian motion. II. Heat transfer and energy partitioning of a free particle. <i>Journal of Chemical Physics</i> , 2018, 149, 104103.	1.2	3
150	Small Dielectric Clusters: Size and Shape Dependence of Photophysical and Photochemical Properties. <i>Jerusalem Symposia on Quantum Chemistry and Biochemistry</i> , 1987, , 333-343.	0.2	1
151	Heat transport induced by electron transfer: A general temperature quantum calculation. <i>Journal of Chemical Physics</i> , 2021, 155, 194104.	1.2	1
152	The Mechanism and Modeling of Conductivity in Polymer Electrolytes. <i>Materials Research Society Symposia Proceedings</i> , 1994, 369, 245.	0.1	0