

Thorsten Hansen

List of Publications by Year in descending order

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58
papers

1,829
citations

361413

20
h-index

265206

42
g-index

61
all docs

61
docs citations

61
times ranked

1971
citing authors

#	ARTICLE	IF	CITATIONS
1	Exploring local currents in molecular junctions. <i>Nature Chemistry</i> , 2010, 2, 223-228.	13.6	375
2	Understanding quantum interference in coherent molecular conduction. <i>Journal of Chemical Physics</i> , 2008, 129, 054701.	3.0	232
3	Quantum Interference in Acyclic Systems: Conductance of Cross-Conjugated Molecules. <i>Journal of the American Chemical Society</i> , 2008, 130, 17301-17308.	13.7	219
4	Interfering pathways in benzene: An analytical treatment. <i>Journal of Chemical Physics</i> , 2009, 131, 194704.	3.0	121
5	Quantum Interference: The Structural Dependence of Electron Transmission through Model Systems and Cross-Conjugated Molecules. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16991-16998.	3.1	63
6	Nonequilibrium steady state transport via the reduced density matrix operator. <i>Journal of Chemical Physics</i> , 2009, 130, 144105.	3.0	52
7	Simple and Accurate Method for Time-Dependent Transport along Nanoscale Junctions. <i>Journal of Physical Chemistry C</i> , 2014, 118, 20009-20017.	3.1	41
8	Parameter-free driven Liouville-von Neumann approach for time-dependent electronic transport simulations in open quantum systems. <i>Journal of Chemical Physics</i> , 2017, 146, 092331.	3.0	40
9	Charge transfer excitation energies in pyridine-silver complexes studied by a QM/MM method. <i>Chemical Physics Letters</i> , 2009, 470, 285-288.	2.6	38
10	Gated-Controlled Rectification of a Self-Assembled Monolayer-Based Transistor. <i>Journal of Physical Chemistry C</i> , 2013, 117, 8468-8474.	3.1	38
11	Controlling Two-Step Multimode Switching of Dihydroazulene Photoswitches. <i>Chemistry - A European Journal</i> , 2015, 21, 3968-3977.	3.3	36
12	Tracking molecular resonance forms of donor-acceptor push-pull molecules by single-molecule conductance experiments. <i>Nature Communications</i> , 2015, 6, 10233.	12.8	36
13	3D Spectroscopy of Vibrational Coherences in Quantum Dots: Theory. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11124-11133.	2.6	33
14	Understanding and Controlling Crosstalk between Parallel Molecular Wires. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1667-1671.	4.6	32
15	Multireference Excitation Energies for Bacteriochlorophylls A within Light Harvesting System 2. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1305-1313.	5.3	32
16	Communication: Finding destructive interference features in molecular transport junctions. <i>Journal of Chemical Physics</i> , 2014, 141, 181103.	3.0	30
17	Orbital Topology Controlling Charge Injection in Quantum-Dot-Sensitized Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1157-1162.	4.6	27
18	Absorption and Fluorescence Lineshape Theory for Polynomial Potentials. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5979-5989.	5.3	27

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19	Molecular Transport Junctions with Semiconductor Electrodes: Analytical Forms for One-Dimensional Self-Energies. <i>Journal of Physical Chemistry A</i> , 2009, 113, 4665-4676.	2.5	22
20	Macrocycle ring deformation as the secondary design principle for light-harvesting complexes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E9051-E9057.	7.1	21
21	Frequency-Dependent Polarizabilities of Amino Acids as Calculated by an Electrostatic Interaction Model. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 626-633.	5.3	20
22	Nature of relaxation processes revealed by the action signals of intensity-modulated light fields. <i>Physical Review A</i> , 2016, 94, .	2.5	19
23	Intermolecular Modes between LH2 Bacteriochlorophylls and Protein Residues: The Effect on the Excitation Energies. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5499-5508.	2.6	19
24	Polarizability as a Molecular Descriptor for Conductance in Organic Molecular Circuits. <i>Journal of Physical Chemistry C</i> , 2016, 120, 26054-26060.	3.1	16
25	Nonlinear Optical Effects Induced by Nanoparticles in Symmetric Molecules. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20870-20876.	3.1	15
26	Q_{xy} and Q_{xx} Absorption Bands for Bacteriochlorophyll a Molecules from LH2 and LH3. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5283-5292.	2.5	15
27	Classification of dark states in multilevel dissipative systems. <i>Physical Review A</i> , 2019, 99, .	2.5	15
28	Band Gap Energy of Gradient Core-Shell Quantum Dots. <i>Journal of Physical Chemistry C</i> , 2017, 121, 13655-13659.	3.1	14
29	Two-dimensional electronic spectroscopy of anharmonic molecular potentials. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 1642-1652.	2.8	14
30	Computational assignment of redox states to Coulomb blockade diamonds. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 17473-17478.	2.8	11
31	Adiabatic elimination and subspace evolution of open quantum systems. <i>Physical Review A</i> , 2020, 101, .	2.5	11
32	Cotunneling Model for Current-Induced Events in Molecular Wires. <i>Nano Letters</i> , 2008, 8, 3525-3531.	9.1	10
33	Boron Subphthalocyanine Based Molecular Triad Systems for the Capture of Solar Energy. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7694-7703.	2.5	10
34	Excited-State Topology Modifications of the Dihydroazulene Photoswitch Through Aromaticity. <i>ChemPhotoChem</i> , 2019, 3, 619-629.	3.0	10
35	A theoretical approach to molecular single-electron transistors. <i>Theoretical Chemistry Accounts</i> , 2011, 130, 839-850.	1.4	9
36	Interatomic inelastic current. <i>Journal of Chemical Physics</i> , 2017, 146, 092322.	3.0	9

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37	A molecule wired: Electrostatic investigation. <i>Chemical Physics Letters</i> , 2005, 405, 118-122.	2.6	8
38	Nonlinear response theory on the Keldysh contour. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2012, 45, 154014.	1.5	8
39	Coherent two-dimensional spectroscopy of a Fano model. <i>Physical Review B</i> , 2016, 94, .	3.2	8
40	Molecular properties of molecules between electrodes. <i>Theoretical Chemistry Accounts</i> , 2004, 111, 122-131.	1.4	7
41	Drastic difference between hole and electron injection through the gradient shell of Cd _x Se _y Zn _{1-x} S _y quantum dots. <i>Nanoscale</i> , 2017, 9, 12503-12508.	5.6	7
42	Molecular Properties of Sandwiched Molecules Between Electrodes and Nanoparticles. <i>Advances in Quantum Chemistry</i> , 2017, 75, 53-102.	0.8	7
43	Dark Photoswitching Induces Coulomb Blockade Diamond Collapse. <i>Journal of Physical Chemistry C</i> , 2015, 119, 14829-14833.	3.1	6
44	Subphthalocyanine-radiannulene scaffold as a multi-electron acceptor and strong chromophore. <i>Chemical Communications</i> , 2018, 54, 2763-2766.	4.1	6
45	Two-dimensional Fano lineshapes: Excited-state absorption contributions. <i>Journal of Chemical Physics</i> , 2018, 148, 184201.	3.0	6
46	Spectral shifts of BODIPY derivatives: a simple continuous model. <i>Photochemical and Photobiological Sciences</i> , 2019, 18, 1315-1323.	2.9	5
47	Hole Hopping through Cytochrome P450. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3065-3073.	2.6	5
48	The chemistry of Coulomb blockade diamonds for 1,4-diamino-benzene. <i>Chemical Physics</i> , 2015, 459, 40-44.	1.9	3
49	Stepwise "Dark Photoswitching" of Photochromic Dimers in a Junction. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3163-3170.	3.1	3
50	Conformationally controlled ultrafast intersystem crossing in bithiophene systems. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 13412-13418.	2.8	3
51	Computational construction of the electronic Hamiltonian for photoinduced electron transfer and Redfield propagation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17366-17377.	2.8	3
52	Predicting transport regime and local electrostatic environment from Coulomb blockade diamond sizes. <i>Journal of Chemical Physics</i> , 2017, 146, 104306.	3.0	2
53	A Study of Electrocyclic Reactions in a Molecular Junction: Mechanistic and Energetic Requirements for Switching in the Coulomb Blockade Regime. <i>ChemPhysChem</i> , 2017, 18, 1517-1525.	2.1	2
54	Excited-State Topology Modifications of the Dihydroazulene Photoswitch Through Aromaticity. <i>ChemPhotoChem</i> , 2019, 3, 577.	3.0	2

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55	The Sulfolene Protecting Group: Observation of a Direct Photoinitiated Cheletropic Ring Opening. ChemPhotoChem, 2021, 5, 863-870.	3.0	1
56	Predicting slow relaxation timescales in open quantum systems. Journal of Mathematical Chemistry, 2022, 60, 1542-1554.	1.5	1
57	Non-Adiabatic Effects in Electron Tunneling in Molecular Junctions. AIP Conference Proceedings, 2007, , .	0.4	0
58	A Study of Electrocyclic Reactions in a Molecular Junction: Mechanistic and Energetic Requirements for Switching in the Coulomb Blockade Regime. ChemPhysChem, 2017, 18, 1492-1492.	2.1	0