

Thomas Frederiksen

List of Publications by Year in descending order

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80
papers

3,749
citations

172207

29
h-index

128067

60
g-index

81
all docs

81
docs citations

81
times ranked

3366
citing authors

#	ARTICLE	IF	CITATIONS
1	Inelastic transport theory from first principles: Methodology and application to nanoscale devices. <i>Physical Review B</i> , 2007, 75, .	1.1	378
2	Improvements on non-equilibrium and transport Green function techniques: The next-generation transiesta. <i>Computer Physics Communications</i> , 2017, 212, 8-24.	3.0	256
3	Inelastic Scattering and Local Heating in Atomic Gold Wires. <i>Physical Review Letters</i> , 2004, 93, 256601.	2.9	204
4	Modeling inelastic phonon scattering in atomic- and molecular-wire junctions. <i>Physical Review B</i> , 2005, 72, .	1.1	192
5	Unified Description of Inelastic Propensity Rules for Electron Transport through Nanoscale Junctions. <i>Physical Review Letters</i> , 2008, 100, 226604.	2.9	181
6	Conductance of Alkanedithiol Single-Molecule Junctions: A Molecular Dynamics Study. <i>Nano Letters</i> , 2009, 9, 117-121.	4.5	153
7	Single spin localization and manipulation in graphene open-shell nanostructures. <i>Nature Communications</i> , 2019, 10, 200.	5.8	134
8	Inelastic Transport through Molecules: Comparing First-Principles Calculations to Experiments. <i>Nano Letters</i> , 2006, 6, 258-262.	4.5	133
9	Atomic-scale engineering of electrodes for single-molecule contacts. <i>Nature Nanotechnology</i> , 2011, 6, 23-27.	15.6	128
10	Controlled Contact to a C ₆₀ Molecule. <i>Physical Review Letters</i> , 2007, 98, 065502.	2.9	126
11	Uncovering the Triplet Ground State of Triangular Graphene Nanoflakes Engineered with Atomic Precision on a Metal Surface. <i>Physical Review Letters</i> , 2020, 124, 177201.	2.9	113
12	Force-induced tautomerization in a single molecule. <i>Nature Chemistry</i> , 2016, 8, 935-940.	6.6	111
13	H-atom relay reactions in real space. <i>Nature Materials</i> , 2012, 11, 167-172.	13.3	105
14	Passing Current through Touching Molecules. <i>Physical Review Letters</i> , 2009, 103, 206803.	2.9	104
15	Action spectroscopy for single-molecule reactions – Experiments and theory. <i>Progress in Surface Science</i> , 2015, 90, 85-143.	3.8	93
16	Magnetism of Topological Boundary States Induced by Boron Substitution in Graphene Nanoribbons. <i>Physical Review Letters</i> , 2020, 125, 146801.	2.9	73
17	Topological phase transition in chiral graphene nanoribbons: from edge bands to end states. <i>Nature Communications</i> , 2021, 12, 5538.	5.8	66
18	On-Surface Synthesis and Collective Spin Excitations of a Triangulene-Based Nanostar. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 25224-25229.	7.2	66

#	ARTICLE	IF	CITATIONS
19	Charge Transport in Azobenzene-Based Single-Molecule Junctions. <i>Physical Review Letters</i> , 2012, 109, 226801.	2.9	64
20	From tunneling to contact: Inelastic signals in an atomic gold junction from first principles. <i>Physical Review B</i> , 2007, 75, .	1.1	56
21	Exploring the Tilt-Angle Dependence of Electron Tunneling across Molecular Junctions of Self-Assembled Alkanethiols. <i>ACS Nano</i> , 2009, 3, 2073-2080.	7.3	53
22	Dynamic Jahn-Teller effect in electronic transport through single C ₆₀ molecules. <i>Physical Review B</i> , 2008, 78, .	1.1	51
23	Efficient calculation of inelastic vibration signals in electron transport: Beyond the wide-band approximation. <i>Physical Review B</i> , 2014, 89, .	1.1	51
24	Characterization of single-molecule pentanedithiol junctions by inelastic electron tunneling spectroscopy and first-principles calculations. <i>Physical Review B</i> , 2010, 81, .	1.1	47
25	Force and conductance during contact formation to a C ₆₀ molecule. <i>New Journal of Physics</i> , 2012, 14, 073032.	1.2	46
26	Surveying Molecular Vibrations during the Formation of Metal-Molecule Nanocontacts. <i>Nano Letters</i> , 2010, 10, 657-660.	4.5	45
27	Simulation of inelastic electron tunneling spectroscopy of single molecules with functionalized tips. <i>Physical Review B</i> , 2011, 83, .	1.1	33
28	Inelastic shot noise characteristics of nanoscale junctions from first principles. <i>Physical Review B</i> , 2012, 86, .	1.1	30
29	Submolecular Resolution by Variation of the Inelastic Electron Tunneling Spectroscopy Amplitude and its Relation to the AFM/STM Signal. <i>Physical Review Letters</i> , 2017, 119, 166001.	2.9	30
30	Theory of action spectroscopy for single-molecule reactions induced by vibrational excitations with STM. <i>Physical Review B</i> , 2014, 89, .	1.1	29
31	Electronic transport in planar atomic-scale structures measured by two-probe scanning tunneling spectroscopy. <i>Nature Communications</i> , 2019, 10, 1573.	5.8	29
32	Magnetic Interactions Between Radical Pairs in Chiral Graphene Nanoribbons. <i>Nano Letters</i> , 2022, 22, 164-171.	4.5	29
33	Inelastic quantum transport in nanostructures: The self-consistent Born approximation and correlated electron-ion dynamics. <i>Physical Review B</i> , 2008, 78, .	1.1	27
34	Engineering Negative Differential Conductance with the Cu(111) Surface State. <i>Physical Review Letters</i> , 2011, 107, 246801.	2.9	27
35	Strong electron-phonon coupling in the π band of graphene. <i>Physical Review B</i> , 2017, 95, .	1.1	27
36	Conductance of a Freestanding Conjugated Molecular Wire. <i>Physical Review Letters</i> , 2017, 119, 066801.	2.9	27

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37	On the mechanical and electronic properties of thiolated gold nanocrystals. <i>Nanoscale</i> , 2015, 7, 1809-1819.	2.8	23
38	Chemical control of electrical contact to sp ² carbon atoms. <i>Nature Communications</i> , 2014, 5, 3659.	5.8	22
39	Electron Transport in Nanoporous Graphene: Probing the Talbot Effect. <i>Nano Letters</i> , 2019, 19, 576-581.	4.5	22
40	Single-Photon Emission Mediated by Single-Electron Tunneling in Plasmonic Nanojunctions. <i>Physical Review Letters</i> , 2019, 123, 246601.	2.9	20
41	Controlling single-molecule junction conductance by molecular interactions. <i>Scientific Reports</i> , 2015, 5, 11796.	1.6	19
42	Atomic-scale characterization of the interfacial phonon in graphene/SiC. <i>Physical Review B</i> , 2017, 96, .	1.1	19
43	A tunable electronic beam splitter realized with crossed graphene nanoribbons. <i>Journal of Chemical Physics</i> , 2017, 146, 092318.	1.2	18
44	The butterfly “ a well-defined constant-current topography pattern on Si(001):H and Ge(001):H resulting from current-induced defect fluctuations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 19309-19317.	1.3	16
45	Rotation of Ethoxy and Ethyl Moieties on a Molecular Platform on Au(111). <i>ACS Nano</i> , 2020, 14, 3907-3916.	7.3	15
46	Normal-superconducting phase transition mimicked by current noise. <i>Physical Review B</i> , 2004, 70, .	1.1	14
47	Identification of pristine and defective graphene nanoribbons by phonon signatures in the electron transport characteristics. <i>Physical Review B</i> , 2015, 91, .	1.1	14
48	Modeling of Inelastic Transport in One-Dimensional Metallic Atomic Wires. <i>Journal of Computational Electronics</i> , 2004, 3, 423-427.	1.3	13
49	Vibrationally induced flip motion of a hydroxyl dimer on Cu(110). <i>Physical Review B</i> , 2011, 84, .	1.1	13
50	Interface Dipole Effects as a Function of Molecular Tilt: Mechanical Gating of Electron Tunneling through Self-Assembled Monolayers?. <i>Journal of Physical Chemistry C</i> , 2013, 117, 14272-14280.	1.5	12
51	Role of valence states of adsorbates in inelastic electron tunneling spectroscopy: A study of nitric oxide on Cu(110) and Cu(001). <i>Physical Review B</i> , 2016, 94, .	1.1	12
52	Phonon scattering in nanoscale systems: lowest order expansion of the current and power expressions. <i>Journal of Physics: Conference Series</i> , 2006, 35, 247-254.	0.3	11
53	Tunneling spectroscopy of close-spaced dangling-bond pairs in Si(001):H. <i>Scientific Reports</i> , 2015, 5, 14496.	1.6	11
54	Role of k -point sampling in the supercell approach to inelastic electron tunneling spectroscopy simulations of molecular monolayers. <i>Physical Review B</i> , 2015, 91, .	1.1	11

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55	Search for a Metallic Dangling-Bond Wire on <i>n</i> -Doped H-Passivated Semiconductor Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 20303-20309.	1.5	11
56	Conductance channels of a platform molecule on Au(111) probed with shot noise. <i>Physical Review B</i> , 2019, 99, .	1.1	11
57	Spin-Polarizing Electron Beam Splitter from Crossed Graphene Nanoribbons. <i>Physical Review Letters</i> , 2022, 129, .	2.9	11
58	Identifying Highly Conducting Au-C Links through Inelastic Electron Tunneling Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2014, 118, 27106-27112.	1.5	10
59	Crossed graphene nanoribbons as beam splitters and mirrors for electron quantum optics. <i>Physical Review B</i> , 2020, 102, .	1.1	10
60	Inelastic fingerprints of hydrogen contamination in atomic gold wire systems. <i>Journal of Physics: Conference Series</i> , 2007, 61, 312-316.	0.3	9
61	Controlled switching of single-molecule junctions by mechanical motion of a phenyl ring. <i>Beilstein Journal of Nanotechnology</i> , 2015, 6, 2088-2095.	1.5	9
62	Nonequilibrium electron-vibration coupling and conductance fluctuations in a C ₆₀ junction. <i>Physical Review B</i> , 2012, 86, .	1.1	8
63	Inelastic electron tunneling spectroscopy by STM of phonons at solid surfaces and interfaces. <i>Progress in Surface Science</i> , 2018, 93, 131-145.	3.8	8
64	High-conductance contacts to functionalized molecular platforms physisorbed on Au(111). <i>Journal of Physics Condensed Matter</i> , 2019, 31, 18LT01.	0.7	6
65	Photon-emission statistics induced by electron tunneling in plasmonic nanojunctions. <i>Physical Review B</i> , 2021, 104, .	1.1	6
66	Zero-field superconducting phase transition obscured by finite-size effects in thick YBa ₂ Cu ₃ O _{7-δ} films. <i>Physical Review B</i> , 2004, 69, .	1.1	5
67	Phonon-induced linewidths of graphene electronic states. <i>Physical Review B</i> , 2018, 98, .	1.1	5
68	Effect of adsorbates on single-molecule junction conductance. <i>Surface Science</i> , 2018, 678, 169-176.	0.8	5
69	Bimetallic electrodes boost molecular junctions. <i>Nature Materials</i> , 2021, 20, 577-578.	13.3	5
70	Effects of self field and low magnetic fields on the normal-superconducting phase transition. <i>Physical Review B</i> , 2005, 72, .	1.1	4
71	Publisher's Note: A tunable electronic beam splitter realized with crossed graphene nanoribbons. <i>J. Chem. Phys.</i> 146, 092318 (2017)]. <i>Journal of Chemical Physics</i> , 2017, 146, 199902.	1.2	4
72	Molecular Electronics: Insight from First-Principles Transport Simulations. <i>Chimia</i> , 2010, 64, 350.	0.3	3

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73	Onâ€Surface Synthesis and Collective Spin Excitations of a Trianguleneâ€Based Nanostar. Angewandte Chemie, 0, , .	1.6	3
74	Magnetic-State Controlled Molecular Vibrational Dynamics at Buried Molecularâ€Metal Interfaces. Journal of Physical Chemistry C, 2018, 122, 26499-26505.	1.5	2
75	Nanomechanics of a hydrogen molecule suspended between two equally charged tips. Physical Review B, 2020, 101, .	1.1	1
76	DFT-NEGF Approach to Current-Induced Forces, Vibrational Signals and Heating in Nanoconductors. , 2010, , .		1
77	What a superconducting transition should look like: extrapolating data from scaling plots. Physica C: Superconductivity and Its Applications, 2004, 408-410, 562-563.	0.6	0
78	First-principles Theory of Inelastic Transport and Local Heating in Atomic Gold Wires. AIP Conference Proceedings, 2007, , .	0.3	0
79	Frontispiece: Onâ€Surface Synthesis and Collective Spin Excitations of a Trianguleneâ€Based Nanostar. Angewandte Chemie - International Edition, 2021, 60, .	7.2	0
80	Frontispiz: Onâ€Surface Synthesis and Collective Spin Excitations of a Trianguleneâ€Based Nanostar. Angewandte Chemie, 2021, 133, .	1.6	0