Fabian Pauly

List of Publications by Year
in descending order

84 papers	4,654 citations	101535 36 h-index	95259 68 g-index
88 all docs	88 docs citations	88 times ranked	4054 citing authors

#	Article	IF	Citations
1	Optical rectification and field enhancement in a plasmonic nanogap. Nature Nanotechnology, 2010, 5, 732-736.	31.5	348
2	Highly Conductive Molecular Junctions Based on Direct Binding of Benzene to Platinum Electrodes. Physical Review Letters, 2008, 101, 046801.	7.8	287
3	Influence of Conformation on Conductance of Biphenyl-Dithiol Single-Molecule Contacts. Nano Letters, 2010, 10, 156-163.	9.1	284
4	Heat dissipation in atomic-scale junctions. Nature, 2013, 498, 209-212.	27.8	219
5	Single-Molecule Junctions Based on Nitrile-Terminated Biphenyls: A Promising New Anchoring Group. Journal of the American Chemical Society, 2011, 133, 184-187.	13.7	212
6	Revealing the Role of Anchoring Groups in the Electrical Conduction Through Singleâ€Molecule Junctions. Small, 2010, 6, 1529-1535.	10.0	200
7	Quantized thermal transport in single-atom junctions. Science, 2017, 355, 1192-1195.	12.6	165
8	Charge Transport Characteristics of Diarylethene Photoswitching Single-Molecule Junctions. Nano Letters, 2012, 12, 3736-3742.	9.1	163
9	Electron-vibration interaction in transport through atomic gold wires. Physical Review B, 2005, 72, .	3.2	161
10	Structure and conductance histogram of atomic-sized Au contacts. Physical Review B, 2005, 72, .	3.2	134
11	Thermal conductance of single-molecule junctions. Nature, 2019, 572, 628-633.	27.8	127
12	A current-driven single-atom memory. Nature Nanotechnology, 2013, 8, 645-648.	31.5	119
13	Length-dependent conductance and thermopower in single-molecule junctions of dithiolated oligophenylene derivatives: A density functional study. Physical Review B, 2008, 78, .	3.2	112
14	Theoretical analysis of the conductance histograms and structural properties of Ag, Pt, and Ni nanocontacts. Physical Review B, 2006, 74, .	3.2	95
15	Influence of Quantum Interference on the Thermoelectric Properties of Molecular Junctions. Nano Letters, 2018, 18, 5666-5672.	9.1	93
16	Density-functional study of tilt-angle and temperature-dependent conductance in biphenyl dithiol single-molecule junctions. Physical Review B, 2008, 77, .	3.2	91
17	Characteristics of Amine-Ended and Thiol-Ended Alkane Single-Molecule Junctions Revealed by Inelastic Electron Tunneling Spectroscopy. ACS Nano, 2011, 5, 4104-4111.	14.6	90
18	Heat dissipation and its relation to thermopower in single-molecule junctions. New Journal of Physics, 2014, 16, 015004.	2.9	88

#	Article	IF	Citations
19	Theoretical description of the electrical conduction in atomic and molecular junctions. Nanotechnology, 2003, 14, R29-R38.	2.6	85
20	Electric Transport Properties of Surface-Anchored Metalâ€“Organic Frameworks and the Effect of Ferrocene Loading. ACS Applied Materials & Interfaces, 2015, 7, 9824-9830.	8.0	83
21	Cluster-based density-functional approach to quantum transport through molecular and atomic contacts. New Journal of Physics, 2008, 10, 125019.	2.9	82
22	Conduction mechanisms in biphenyl dithiol single-molecule junctions. Physical Review B, 2012, 85, .	3.2	82
23	An electrically actuated molecular toggle switch. Nature Communications, 2017, 8, 14672.	12.8	77
24	Large Conductance Variations in a Mechanosensitive Single-Molecule Junction. Nano Letters, 2018, 18, 5981-5988.	9.1	69
25	Modeling elastic and photoassisted transport in organic molecular wires: Length dependence and current-voltage characteristics. Physical Review B, 2008, 77, .	3.2	58
26	Plasmon-Induced Conductance Enhancement in Single-Molecule Junctions. Journal of Physical Chemistry Letters, 2013, 4, 2811-2816.	4.6	58
27	First-principles calculation of the thermoelectric figure of merit for [2,2]paracyclophane-based single-molecule junctions. Physical Review B, 2015, 91, .	3.2	54
28	Theoretical study of the charge transport through C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>60</mml:mn></mml:msub></mml:math>-based single-molecule junctions. Physical Review B, 2012, 85, .	3.2	51
29	Highly Ordered Surface Self-Assembly of Fe4 Single Molecule Magnets. Nano Letters, 2015, 15, 4546-4552.	9.1	50
30	Shot Noise of 1,4-Benzenedithiol Single-Molecule Junctions. Nano Letters, 2016, 16, 1803-1807.	9.1	44
31	<i>Ab initio</i>study of the thermopower of biphenyl-based single-molecule junctions. Physical Review B, 2012, 86, .	3.2	43
32	Theoretical study of the conductance of ferromagnetic atomic-sized contacts. Physical Review B, 2008, 77, .	3.2	42
33	Molecular dynamics study of the thermopower of Ag, Au, and Pt nanocontacts. Physical Review B, 2011, 84, .	3.2	41
34	Length dependence of the thermal conductance of alkane-based single-molecule junctions: An<i>ab initio</i>study. Physical Review B, 2016, 94, .	3.2	40
35	Quantum Thermopower of Metallic Atomic-Size Contacts at Room Temperature. Nano Letters, 2015, 15, 1006-1011.	9.1	39
36	Photoconductance of organic single-molecule contacts. Physical Review B, 2007, 76, .	3.2	37

#	Article	IF	Citations
37	Thermal conductance and thermoelectric figure of merit of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math> -based single-molecule junctions: Electrons, phonons, and photons. Physical Review B, 2017, 95, .	3.2	36
38	Tuning the thermal conductance of molecular junctions with interference effects. Physical Review B, 2017, 96, .	3.2	31
39	Redoxâ€Active Tetraruthenium Macrocycles Built from 1,4â€Divinylphenyleneâ€Bridged Diruthenium Complexes. Chemistry - A European Journal, 2016, 22, 9574-9590.	3.3	30
40	Single-molecule conductance of a chemically modified, Ï€-extended tetrathiafulvalene and its charge-transfer complex with F₄TCNQ. Beilstein Journal of Organic Chemistry, 2015, 11, 1068-1078.	2.2	29
41	Influence of vibrations on electron transport through nanoscale contacts. Physica Status Solidi (B): Basic Research, 2013, 250, 2468-2480.	1.5	26
42	Identification of the current path for a conductive molecular wire on a tripodal platform. Nanoscale, 2016, 8, 10582-10590.	5.6	24
43	Substitution Pattern Controlled Quantum Interference in [2.2]Paracyclophane-Based Single-Molecule Junctions. Journal of the American Chemical Society, 2021, 143, 13944-13951.	13.7	24
44	Thermal conductance of metallic atomic-size contacts: Phonon transport and Wiedemann-Franz law. Physical Review B, 2017, 96, .	3.2	23
45	Unidirectional Real-Time Photoswitching of Diarylethene Molecular Monolayer Junctions with Multilayer Graphene Electrodes. ACS Applied Materials & Interfaces, 2019, 11, 11645-11653.	8.0	23
46	Conductance of atomic-scale Pb contacts in an electrochemical environment. Physical Review B, 2010, 82, .	3.2	22
47	Charge Transport through Ferrocene 1,1â€²â€Diamine Singleâ€Molecule Junctions. Small, 2016, 12, 4849-4856.	10.0	19
48	Control of excitonic absorption by thickness variation in few-layer GaSe. Physical Review B, 2019, 100, .	3.2	19
49	Plasmon polaritons in cubic lattices of spherical metallic nanoparticles. Physical Review B, 2018, 97, .	3.2	18
50	Harnessing Excitonâ€“Exciton Annihilation in Two-Dimensional Semiconductors. Nano Letters, 2020, 20, 1647-1653.	9.1	18
51	Robust Periodic Fock Exchange with Atom-Centered Gaussian Basis Sets. Journal of Chemical Theory and Computation, 2018, 14, 4567-4580.	5.3	17
52	The conduction properties of Î±,Ï‰-diaminoalkanes and hydrazine bridging gold electrodes. Chemical Physics Letters, 2008, 454, 284-288.	2.6	16
53	Raman Scattering from a Moleculeâ€“Semiconductor Interface Tuned by an Electric Field: Density Functional Theory Approach. Journal of Physical Chemistry C, 2015, 119, 23113-23118.	3.1	16
54	Transmission eigenchannels for coherent phonon transport. Physical Review B, 2018, 97, .	3.2	16

#	Article	IF	Citations
55	Electric-field control of single-molecule tautomerization. Physical Chemistry Chemical Physics, 2020, 22, 6370-6375.	2.8	16
56	<i>Ab initio</i>study of charge transport through single oxygen molecules in atomic aluminum contacts. Physical Review B, 2007, 76, .	3.2	15
57	Charge transport in a single molecule transistor probed by scanning tunneling microscopy. Nanoscale, 2018, 10, 1487-1493.	5.6	14
58	Copper(I)-Based Flexible Organicâ€“Inorganic Coordination Polymer and Analogues: High-Power Factor Thermoelectrics. ACS Applied Materials & Interfaces, 2020, 12, 53841-53851.	8.0	14
59	Shot noise variation within ensembles of gold atomic break junctions at room temperature. Journal of Physics Condensed Matter, 2014, 26, 474204.	1.8	12
60	Inelastic electron tunneling spectroscopy of difurylethene-based photochromic single-molecule junctions. Beilstein Journal of Nanotechnology, 2017, 8, 2606-2614.	2.8	11
61	Effect of Charge-Assisted Hydrogen Bonds on Single-Molecule Electron Transport. Journal of Physical Chemistry C, 2019, 123, 29386-29393.	3.1	11
62	Dynamical Coulomb Blockade as a Local Probe for Quantum Transport. Physical Review Letters, 2020, 124, 156803.	7.8	11
63	Doping hepta-alanine with tryptophan: A theoretical study of its effect on the electrical conductance of peptide-based single-molecule junctions. Journal of Chemical Physics, 2019, 150, 174705.	3.0	10
64	Voltage-Induced Rearrangements in Atomic-Size Contacts. Nano Letters, 2020, 20, 5773-5778.	9.1	10
65	Mechanical conductance tunability of a porphyrinâ€“cyclophane single-molecule junction. Nanoscale, 2022, 14, 984-992.	5.6	10
66	Conduction channels of one-atom zinc contacts. Physical Review B, 2004, 70, .	3.2	9
67	Multiplicity of atomic reconfigurations in an electrochemical Pb single-atom transistor. Physical Review B, 2017, 95, .	3.2	8
68	Thermalization of photoexcited carriers in two-dimensional transition metal dichalcogenides and internal quantum efficiency of van der Waals heterostructures. Physical Review Research, 2020, 2, .	3.6	8
69	Mechanical compression in cofacial porphyrin cyclophane pincers. Chemical Science, 2022, 13, 8017-8024.	7.4	7
70	Charge-carrier thermalization in bulk and monolayer CdTe from first principles. Physical Review B, 2021, 103, .	3.2	6
71	Towards a theory of electrical transport through atomic and molecular junctions. Phase Transitions, 2004, 77, 175-189.	1.3	5
72	Giant anisotropic magnetoresistance through a tilted molecular <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï€</mml:mi></mml:math> -orbital. Physical Review Research, 2020, 2, .	3.6	5

#	Article	IF	Citations
73	Two-dimensional, phenanthroline-based, extended Ï€-conjugated molecules for single-molecule conduction. Journal of Physics Condensed Matter, 2008, 20, 295208.	1.8	4
74	Structural Asymmetry of Metallic Single-Atom Contacts Detected by Currentâ€“Voltage Characteristics. ACS Applied Materials & Interfaces, 2022, 14, 11919-11926.	8.0	4
75	Extracting transport channel transmissions in scanning tunneling microscopy using superconducting excess current. Physical Review B, 2022, 105, .	3.2	4
76	Statistical analysis of electronic and phononic transport simulations of metallic atomic contacts. Physical Review B, 2019, 100, .	3.2	3
77	Tipâ€Induced Inversion of the Chirality of a Molecule's Adsorption Potential Probed by the Switching Directionality. Advanced Materials, 2020, 32, 1907390.	21.0	3
78	Quantum-correlated photons generated by nonlocal electron transport. Physical Review B, 2022, 105, .	3.2	3
79	High-modulation-depth effects in photorefractive wave mixing: influence on pattern formation and physical foundations. Optics Communications, 2003, 218, 385-407.	2.1	2
80	Electronic transport through single noble gas atoms. Physical Review B, 2011, 84, .	3.2	2
81	Plasmons in nanoscale metal junctions: optical rectification and thermometry. , 2011, , .		2
82	Multipole-based distance-dependent screening of Coulomb integrals. Journal of Chemical Physics, 2019, 151, 084111.	3.0	2
83	Thermoelectric Transport from First-Principlesâ€"Biphenyl-Based Single-Molecule Junctions. , 2016, , 43-51.		0
84	Phonon-assisted carrier cooling in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>h</mml:mi></mml:math> -BN/graphene van der Waals heterostructures. Physical Review B, 2022, 105, .	3.2	0