Fabian Pauly

List of Publications by Year
in descending order

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84	4,654	116194	107981
papers	citations	36 h-index	68 g-index

88	88	88	4605
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mechanical conductance tunability of a porphyrinâ€“cyclophane single-molecule junction. Nanoscale, 2022, 14, 984-992.	2.8	10
2	Structural Asymmetry of Metallic Single-Atom Contacts Detected by Currentâ€“Voltage Characteristics. ACS Applied Materials & Interfaces, 2022, 14, 11919-11926.	4.0	4
3	Extracting transport channel transmissions in scanning tunneling microscopy using superconducting excess current. Physical Review B, 2022, 105, .	1.1	4
4	Mechanical compression in cofacial porphyrin cyclophane pincers. Chemical Science, 2022, 13, 8017-8024.	3.7	7
5	Quantum-correlated photons generated by nonlocal electron transport. Physical Review B, 2022, 105, .	1.1	3
6	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, .	1.1	0
7	Charge-carrier thermalization in bulk and monolayer CdTe from first principles. Physical Review B, 2021, 103, .	1.1	6
8	Substitution Pattern Controlled Quantum Interference in [2.2]Paracyclophane-Based Single-Molecule Junctions. Journal of the American Chemical Society, 2021, 143, 13944-13951.	6.6	24
9	Copper(I)-Based Flexible Organicâ€“Inorganic Coordination Polymer and Analogues: High-Power Factor Thermoelectrics. ACS Applied Materials & Interfaces, 2020, 12, 53841-53851.	4.0	14
10	Voltage-Induced Rearrangements in Atomic-Size Contacts. Nano Letters, 2020, 20, 5773-5778.	4.5	10
11	Electric-field control of single-molecule tautomerization. Physical Chemistry Chemical Physics, 2020, 22, 6370-6375.	1.3	16
12	Tipâ€Induced Inversion of the Chirality of a Molecule's Adsorption Potential Probed by the Switching Directionality. Advanced Materials, 2020, 32, 1907390.	11.1	3
13	Harnessing Excitonâ€“Exciton Annihilation in Two-Dimensional Semiconductors. Nano Letters, 2020, 20, 1647-1653.	4.5	18
14	Dynamical Coulomb Blockade as a Local Probe for Quantum Transport. Physical Review Letters, 2020, 124, 156803.	2.9	11
15	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, .	1.3	5
16	Thermalization of photoexcited carriers in two-dimensional transition metal dichalcogenides and internal quantum efficiency of van der Waals heterostructures. Physical Review Research, 2020, 2, .	1.3	8
17	Control of excitonic absorption by thickness variation in few-layer GaSe. Physical Review B, 2019, 100, .	1.1	19
18	Thermal conductance of single-molecule junctions. Nature, 2019, 572, 628-633.	13.7	127

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19	Effect of Charge-Assisted Hydrogen Bonds on Single-Molecule Electron Transport. Journal of Physical Chemistry C, 2019, 123, 29386-29393.	1.5	11
20	Multipole-based distance-dependent screening of Coulomb integrals. Journal of Chemical Physics, 2019, 151, 084111.	1.2	2
21	Statistical analysis of electronic and phononic transport simulations of metallic atomic contacts. Physical Review B, 2019, 100, .	1.1	3
22	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.	1.2	10
23	Unidirectional Real-Time Photoswitching of Diarylethene Molecular Monolayer Junctions with Multilayer Graphene Electrodes. ACS Applied Materials & Interfaces, 2019, 11, 11645-11653.	4.0	23
24	Transmission eigenchannels for coherent phonon transport. Physical Review B, 2018, 97, .	1.1	16
25	Charge transport in a single molecule transistor probed by scanning tunneling microscopy. Nanoscale, 2018, 10, 1487-1493.	2.8	14
26	Plasmon polaritons in cubic lattices of spherical metallic nanoparticles. Physical Review B, 2018, 97, .	1.1	18
27	Robust Periodic Fock Exchange with Atom-Centered Gaussian Basis Sets. Journal of Chemical Theory and Computation, 2018, 14, 4567-4580.	2.3	17
28	Influence of Quantum Interference on the Thermoelectric Properties of Molecular Junctions. Nano Letters, 2018, 18, 5666-5672.	4.5	93
29	Large Conductance Variations in a Mechanosensitive Single-Molecule Junction. Nano Letters, 2018, 18, 5981-5988.	4.5	69
30	Quantized thermal transport in single-atom junctions. Science, 2017, 355, 1192-1195.	6.0	165
31	An electrically actuated molecular toggle switch. Nature Communications, 2017, 8, 14672.	5.8	77
32	Multiplicity of atomic reconfigurations in an electrochemical Pb single-atom transistor. Physical Review B, 2017, 95, .	1.1	8
33	Thermal conductance of metallic atomic-size contacts: Phonon transport and Wiedemann-Franz law. Physical Review B, 2017, 96, .	1.1	23
34	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, .	1.1	36
35	Tuning the thermal conductance of molecular junctions with interference effects. Physical Review B, 2017, 96, .	1.1	31
36	Inelastic electron tunneling spectroscopy of difurylethene-based photochromic single-molecule junctions. Beilstein Journal of Nanotechnology, 2017, 8, 2606-2614.	1.5	11

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37	Redoxâ€Active Tetraruthenium Macrocycles Built from 1,4â€Divinylphenyleneâ€Bridged Diruthenium Complexes. Chemistry - A European Journal, 2016, 22, 9574-9590.	1.7	30
38	Identification of the current path for a conductive molecular wire on a tripodal platform. Nanoscale, 2016, 8, 10582-10590.	2.8	24
39	Length dependence of the thermal conductance of alkane-based single-molecule junctions: Anab initiostudy. Physical Review B, 2016, 94, .	1.1	40
40	Charge Transport through Ferrocene 1,1â€²â€Diamine Singleâ€Molecule Junctions. Small, 2016, 12, 4849-4856.	5.2	19
41	Shot Noise of 1,4-Benzenedithiol Single-Molecule Junctions. Nano Letters, 2016, 16, 1803-1807.	4.5	44
42	Thermoelectric Transport from First-Principlesâ€"Biphenyl-Based Single-Molecule Junctions. , 2016, , 43-51.		0
43	First-principles calculation of the thermoelectric figure of merit for [2,2]paracyclophane-based single-molecule junctions. Physical Review B, 2015, 91, .	1.1	54
44	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.	1.3	29
45	Quantum Thermopower of Metallic Atomic-Size Contacts at Room Temperature. Nano Letters, 2015, 15, 1006-1011.	4.5	39
46	Highly Ordered Surface Self-Assembly of Fe4 Single Molecule Magnets. Nano Letters, 2015, 15, 4546-4552.	4.5	50
47	Electric Transport Properties of Surface-Anchored Metalâ€"Organic Frameworks and the Effect of Ferrocene Loading. ACS Applied Materials & Interfaces, 2015, 7, 9824-9830.	4.0	83
48	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.	1.5	16
49	Shot noise variation within ensembles of gold atomic break junctions at room temperature. Journal of Physics Condensed Matter, 2014, 26, 474204.	0.7	12
50	Heat dissipation and its relation to thermopower in single-molecule junctions. New Journal of Physics, 2014, 16, 015004.	1.2	88
51	Plasmon-Induced Conductance Enhancement in Single-Molecule Junctions. Journal of Physical Chemistry Letters, 2013, 4, 2811-2816.	2.1	58
52	A current-driven single-atom memory. Nature Nanotechnology, 2013, 8, 645-648.	15.6	119
53	Influence of vibrations on electron transport through nanoscale contacts. Physica Status Solidi (B): Basic Research, 2013, 250, 2468-2480.	0.7	26
54	Heat dissipation in atomic-scale junctions. Nature, 2013, 498, 209-212.	13.7	219

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55	Ab initiostudy of the thermopower of biphenyl-based single-molecule junctions. Physical Review B, 2012, 86, .	1.1	43
56	Charge Transport Characteristics of Diarylethene Photoswitching Single-Molecule Junctions. Nano Letters, 2012, 12, 3736-3742.	4.5	163
57	Conduction mechanisms in biphenyl dithiol single-molecule junctions. Physical Review B, 2012, 85, .	1.1	82
58	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, .	1.1	51
59	Characteristics of Amine-Ended and Thiol-Ended Alkane Single-Molecule Junctions Revealed by Inelastic Electron Tunneling Spectroscopy. ACS Nano, 2011, 5, 4104-4111.	7.3	90
60	Single-Molecule Junctions Based on Nitrile-Terminated Biphenyls: A Promising New Anchoring Group. Journal of the American Chemical Society, 2011, 133, 184-187.	6.6	212
61	Molecular dynamics study of the thermopower of Ag, Au, and Pt nanocontacts. Physical Review B, 2011, 84, .	1.1	41
62	Electronic transport through single noble gas atoms. Physical Review B, 2011, 84, .	1.1	2
63	Plasmons in nanoscale metal junctions: optical rectification and thermometry. , 2011, , .		2
64	Revealing the Role of Anchoring Groups in the Electrical Conduction Through Singleâ€Molecule Junctions. Small, 2010, 6, 1529-1535.	5.2	200
65	Optical rectification and field enhancement in a plasmonic nanogap. Nature Nanotechnology, 2010, 5, 732-736.	15.6	348
66	Conductance of atomic-scale Pb contacts in an electrochemical environment. Physical Review B, 2010, 82, .	1.1	22
67	Influence of Conformation on Conductance of Biphenyl-Dithiol Single-Molecule Contacts. Nano Letters, 2010, 10, 156-163.	4.5	284
68	The conduction properties of Î±,Ï‰-diaminoalkanes and hydrazine bridging gold electrodes. Chemical Physics Letters, 2008, 454, 284-288.	1.2	16
69	Density-functional study of tilt-angle and temperature-dependent conductance in biphenyl dithiol single-molecule junctions. Physical Review B, 2008, 77, .	1.1	91
70	Modeling elastic and photoassisted transport in organic molecular wires: Length dependence and current-voltage characteristics. Physical Review B, 2008, 77, .	1.1	58
71	Cluster-based density-functional approach to quantum transport through molecular and atomic contacts. New Journal of Physics, 2008, 10, 125019.	1.2	82
72	Two-dimensional, phenanthroline-based, extended Ï€-conjugated molecules for single-molecule conduction. Journal of Physics Condensed Matter, 2008, 20, 295208.	0.7	4

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73	Length-dependent conductance and thermopower in single-molecule junctions of dithiolated oligophenylene derivatives: A density functional study. Physical Review B, 2008, 78, .	1.1	112
74	Highly Conductive Molecular Junctions Based on Direct Binding of Benzene to Platinum Electrodes. Physical Review Letters, 2008, 101, 046801.	2.9	287
75	Theoretical study of the conductance of ferromagnetic atomic-sized contacts. Physical Review B, 2008, 77, .	1.1	42
76	Ab initiostudy of charge transport through single oxygen molecules in atomic aluminum contacts. Physical Review B, 2007, 76, .	1.1	15
77	Photoconductance of organic single-molecule contacts. Physical Review B, 2007, 76, .	1.1	37
78	Theoretical analysis of the conductance histograms and structural properties of Ag, Pt, and Ni nanocontacts. Physical Review B, 2006, 74, .	1.1	95
79	Electron-vibration interaction in transport through atomic gold wires. Physical Review B, 2005, 72, .	1.1	161
80	Structure and conductance histogram of atomic-sized Au contacts. Physical Review B, 2005, 72, .	1.1	134
81	Conduction channels of one-atom zinc contacts. Physical Review B, 2004, 70, .	1.1	9
82	Towards a theory of electrical transport through atomic and molecular junctions. Phase Transitions, 2004, 77, 175-189.	0.6	5
83	High-modulation-depth effects in photorefractive wave mixing: influence on pattern formation and physical foundations. Optics Communications, 2003, 218, 385-407.	1.0	2
84	Theoretical description of the electrical conduction in atomic and molecular junctions. Nanotechnology, 2003, 14, R29-R38.	1.3	85