Mads Brandbyge

List of Publications by Year
in descending order

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162	15,349	36303 51	17105 122
papers	citations	h-index	g-index

164	164	164	8834
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Density-functional method for nonequilibrium electron transport. Physical Review B, 2002, 65, .	3.2	4,752
2	QuantumATK: an integrated platform of electronic and atomic-scale modelling tools. Journal of Physics Condensed Matter, 2020, 32, 015901.	1.8	771
3	Theoretical study of the nonlinear conductance of Di-thiol benzene coupled to Au(1 1 1) surfaces via thiol and thiolate bonds. Computational Materials Science, 2003, 27, 151-160.	3.0	463
4	Inelastic transport theory from first principles: Methodology and application to nanoscale devices. Physical Review B, 2007, 75, .	3.2	378
5	Theory of Rectification in Tour Wires: The Role of Electrode Coupling. Physical Review Letters, 2002, 89, 138301.	7.8	327
6	Quantized conductance in atom-sized wires between two metals. Physical Review B, 1995, 52, 8499-8514.	3.2	307
7	Transmission eigenchannels from nonequilibrium Greenâ€™s functions. Physical Review B, 2007, 76, .	3.2	276
8	Improvements on non-equilibrium and transport Green function techniques: The next-generation transiesta. Computer Physics Communications, 2017, 212, 8-24.	7.5	256
9	Do Aviramâ^'Ratner Diodes Rectify?. Journal of the American Chemical Society, 2003, 125, 3674-3675.	13.7	237
10	Mechanical deformation of atomic-scale metallic contacts: Structure and mechanisms. Physical Review B, 1998, 57, 3283-3294.	3.2	235
11	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
12	First-principles method for electron-phonon coupling and electron mobility: Applications to two-dimensional materials. Physical Review B, 2016, 93, .	3.2	216
13	TranSIESTA: A Spice for Molecular Electronics. Annals of the New York Academy of Sciences, 2003, 1006, 212-226.	3.8	205
14	Inelastic Scattering and Local Heating in Atomic Gold Wires. Physical Review Letters, 2004, 93, 256601.	7.8	204
15	Organometallic Benzene-Vanadium Wire: A One-Dimensional Half-Metallic Ferromagnet. Physical Review Letters, 2006, 97, 097201.	7.8	202
16	Electronically driven adsorbate excitation mechanism in femtosecond-pulse laser desorption. Physical Review B, 1995, 52, 6042-6056.	3.2	199
17	Conductance eigenchannels in nanocontacts. Physical Review B, 1997, 56, 14956-14959.	3.2	196
18	Modeling inelastic phonon scattering in atomic- and molecular-wire junctions. Physical Review B, 2005, 72, .	3.2	192

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19	Conductance switching in a molecular device: The role of side groups and intermolecular interactions. Physical Review B, 2003, 68, .	3.2	191
20	Unified Description of Inelastic Propensity Rules for Electron Transport through Nanoscale Junctions. Physical Review Letters, 2008, 100, 226604.	7.8	181
21	Apparent Barrier Height in Scanning Tunneling Microscopy Revisited. Physical Review Letters, 1996, 76, 1485-1488.	7.8	180
22	Electron and phonon transport in silicon nanowires: Atomistic approach to thermoelectric properties. Physical Review B, 2009, 79, .	3.2	173
23	Conductance of Alkanedithiol Single-Molecule Junctions: A Molecular Dynamics Study. Nano Letters, 2009, 9, 117-121.	9.1	153
24	Surface-Decorated Silicon Nanowires: A Route to High-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Z</mml:mi><mml:mi>T</mml:mi></mml:math>Thermoelectrics. Physical Review Letters, 2009, 103, 055502.	7.8	149
25	Conduction channels at finite bias in single-atom gold contacts. Physical Review B, 1999, 60, 17064-17070.	3.2	143
26	Electronic properties of graphene antidot lattices. New Journal of Physics, 2009, 11, 095020.	2.9	143
27	General atomistic approach for modeling metal-semiconductor interfaces using density functional theory and nonequilibrium Green's function. Physical Review B, 2016, 93, .	3.2	137
28	Inelastic Transport through Molecules:Â Comparing First-Principles Calculations to Experiments. Nano Letters, 2006, 6, 258-262.	9.1	133
29	Efficient Organometallic Spin Filter between Single-Wall Carbon Nanotube or Graphene Electrodes. Physical Review Letters, 2007, 98, 197202.	7.8	133
30	Thermoelectric properties of finite graphene antidot lattices. Physical Review B, 2011, 84, .	3.2	132
31	Graphene Nanobubbles as Valley Filters and Beam Splitters. Physical Review Letters, 2016, 117, 276801.	7.8	129
32	Controlled Contact to aC60Molecule. Physical Review Letters, 2007, 98, 065502.	7.8	126
33	Electron transport through monovalent atomic wires. Physical Review B, 2004, 69, .	3.2	125
34	First-principles study of electron transport through monatomic Al and Na wires. Physical Review B, 2000, 62, 8430-8437.	3.2	113
35	Scaling Theory Put into Practice: First-Principles Modeling of Transport in Doped Silicon Nanowires. Physical Review Letters, 2007, 99, 076803.	7.8	112
36	Passing Current through Touching Molecules. Physical Review Letters, 2009, 103, 206803.	7.8	104

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37	Blowing the Fuse: Berryâ€™s Phase and Runaway Vibrations in Molecular Conductors. Nano Letters, 2010, 10, 1657-1663.	9.1	103
38	Origin of current-induced forces in an atomic gold wire:â€‚â€‚A first-principles study. Physical Review B, 2003, 67, .	3.2	98
39	Density Functional Simulation of a Breaking Nanowire. Physical Review Letters, 1999, 82, 1538-1541.	7.8	97
40	Current-Voltage Curves of Atomic-Sized Transition Metal Contacts: An Explanation of Why Au is Ohmic and Pt is Not. Physical Review Letters, 2002, 89, 066804.	7.8	95
41	Electronic transport through Si nanowires: Role of bulk and surface disorder. Physical Review B, 2006, 74, .	3.2	95
42	Current-induced atomic dynamics, instabilities, and Raman signals: Quasiclassical Langevin equation approach. Physical Review B, 2012, 85, .	3.2	94
43	Scattering and conductance quantization in three-dimensional metal nanocontacts. Physical Review B, 1997, 55, 2637-2650.	3.2	93
44	Heat Conductance Is Strongly Anisotropic for Pristine Silicon Nanowires. Nano Letters, 2008, 8, 3771-3775.	9.1	90
45	Current-voltage curves of gold quantum point contacts revisited. Applied Physics Letters, 2000, 77, 708-710.	3.3	82
46	Stacked Janus Device Concepts: Abrupt pn-Junctions and Cross-Plane Channels. Nano Letters, 2018, 18, 7275-7281.	9.1	82
47	Atomic-Scale Control of Electron Transport through Single Molecules. Physical Review Letters, 2010, 104, 176802.	7.8	74
48	A two-dimensional Dirac fermion microscope. Nature Communications, 2017, 8, 15783.	12.8	72
49	From tunneling to contact: Inelastic signals in an atomic gold junction from first principles. Physical Review B, 2007, 75, .	3.2	56
50	Density functional study of graphene antidot lattices: Roles of geometrical relaxation and spin. Physical Review B, 2009, 80, .	3.2	56
51	Light Emission Probing Quantum Shot Noise and Charge Fluctuations at a Biased Molecular Junction. Physical Review Letters, 2012, 109, 186601.	7.8	56
52	Exploring the Tilt-Angle Dependence of Electron Tunneling across Molecular Junctions of Self-Assembled Alkanethiols. ACS Nano, 2009, 3, 2073-2080.	14.6	53
53	Piezoresistance in p-type silicon revisited. Journal of Applied Physics, 2008, 104, .	2.5	52
54	Laserlike Vibrational Instability in Rectifying Molecular Conductors. Physical Review Letters, 2011, 107, 046801.	7.8	51

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55	Efficient calculation of inelastic vibration signals in electron transport: Beyond the wide-band approximation. Physical Review B, 2014, 89, .	3.2	51
56	Conductance of single-atom platinum contacts: Voltage dependence of the conductance histogram. Physical Review B, 2003, 67, .	3.2	49
57	Efficient First-Principles Calculation of Phonon-Assisted Photocurrent in Large-Scale Solar-Cell Devices. Physical Review Applied, 2018, 10, .	3.8	49
58	Shot Noise as a Probe of Spin-Polarized Transport through Single Atoms. Physical Review Letters, 2015, 114, 016602.	7.8	46
59	Current-induced forces: a simple derivation. European Journal of Physics, 2014, 35, 065004.	0.6	43
60	First-principles electron transport with phonon coupling: Large scale at low cost. Physical Review B, 2017, 96, .	3.2	41
61	Transmission channels through Na and Al atom wire. Surface Science, 1999, 433-435, 854-857.	1.9	39
62	Simulations of quantum transport in nanoscale systems: application to atomic gold and silver wires. Nanotechnology, 2002, 13, 346-351.	2.6	39
63	Screening model for nanowire surface-charge sensors in liquid. Applied Physics Letters, 2007, 91, .	3.3	39
64	Current-Induced Forces and Hot Spots in Biased Nanojunctions. Physical Review Letters, 2015, 114, 096801.	7.8	39
65	Manipulating the voltage drop in graphene nanojunctions using a gate potential. Physical Chemistry Chemical Physics, 2016, 18, 1025-1031.	2.8	39
66	Ab initiostudy of spin-dependent transport in carbon nanotubes with iron and vanadium adatoms. Physical Review B, 2008, 78, .	3.2	37
67	Quantifying signal changes in nano-wire based biosensors. Nanoscale, 2011, 3, 706-717.	5.6	37
68	Semi-classical generalized Langevin equation for equilibrium and nonequilibrium molecular dynamics simulation. Progress in Surface Science, 2019, 94, 21-40.	8.3	36
69	Theory of the Eigler switch. Physical Review Letters, 1994, 72, 2919-2922.	7.8	35
70	Conductance through Atoms: Dot or Channel?. Japanese Journal of Applied Physics, 1999, 38, 336-338.	1.5	35
71	Predicting and rationalizing the effect of surface charge distribution and orientation on nano-wire based FET bio-sensors. Nanoscale, 2011, 3, 3635.	5.6	35
72	Interface band gap narrowing behind open circuit voltage losses in Cu2ZnSnS4 solar cells. Applied Physics Letters, 2017, 110, .	3.3	35

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73	Modeling Transport in Ultrathin Si Nanowires: Charged versus Neutral Impurities. Nano Letters, 2008, 8, 2825-2828.	9.1	34
74	Localized Edge Vibrations and Edge Reconstruction by Joule Heating in Graphene Nanostructures. Physical Review Letters, 2010, 104, 036807.	7.8	34
75	Electron-phonon scattering from Green's function transport combined with molecular dynamics: Applications to mobility predictions. Physical Review B, 2017, 95, .	3.2	33
76	Spontaneous dissociation of a conjugated molecule on the Si(100) surface. Journal of Chemical Physics, 2002, 117, 321-330.	3.0	32
77	Flexural-Phonon Scattering Induced by Electrostatic Gating in Graphene. Physical Review Letters, 2017, 118, 046601.	7.8	32
78	Electronic transport properties of fullerene functionalized carbon nanotubes:Ab initioand tight-binding calculations. Physical Review B, 2009, 80, .	3.2	30
79	Atomic carbon chains as spin-transmitters: An ab initio transport study. Europhysics Letters, 2010, 91, 37002.	2.0	28
80	Localized electronic states at grain boundaries on the surface of graphene and graphite. 2D Materials, 2016, 3, 031005.	4.4	26
81	Quantum Interference Engineering of Nanoporous Graphene for Carbon Nanocircuitry. Journal of the American Chemical Society, 2019, 141, 13081-13088.	13.7	26
82	Electron and phonon drag in thermoelectric transport through coherent molecular conductors. Physical Review B, 2016, 93, .	3.2	24
83	Current-voltage relation for thin tunnel barriers: Parabolic barrier model. Journal of Applied Physics, 2004, 95, 3582-3586.	2.5	22
84	Electronic and transport properties of kinked graphene. Beilstein Journal of Nanotechnology, 2013, 4, 103-110.	2.8	22
85	Understanding and Engineering Phonon-Mediated Tunneling into Graphene on Metal Surfaces. Nano Letters, 2018, 18, 5697-5701.	9.1	22
86	Electron Transport in Nanoporous Graphene: Probing the Talbot Effect. Nano Letters, 2019, 19, 576-581.	9.1	22
87	Light emission and finite-frequency shot noise in molecular junctions: From tunneling to contact. Physical Review B, 2013, 88, .	3.2	21
88	Field Effect in Graphene-Based van der Waals Heterostructures: Stacking Sequence Matters. Nano Letters, 2017, 17, 2660-2666.	9.1	21
89	A Graphene-Edge Ferroelectric Molecular Switch. Nano Letters, 2018, 18, 4675-4683.	9.1	21
90	Local density of states from transmission amplitudes in multichannel systems. Physical Review B, 1998, 57, R15088-R15091.	3.2	19

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91	Atomistic theory for the damping of vibrational modes in monoatomic gold chains. Physical Review B, 2009, 80, .	3.2	18
92	Phonon excitation and instabilities in biased graphene nanoconstrictions. Physical Review B, 2013, 88, .	3.2	18
93	Unravelling the role of inelastic tunneling into pristine and defected graphene. Physical Review B, 2015, 91, .	3.2	18
94	Unveiling the Multiradical Character of the Biphenylene Network and Its Anisotropic Charge Transport. Journal of the American Chemical Society, 2022, 144, 8278-8285.	13.7	17
95	Ab-initio Non-Equilibrium Greenâ€™s Function Formalism for Calculating Electron Transport in Molecular Devices. , 2006, , 117-151.		16
96	Transport in silicon nanowires: role of radial dopant profile. Journal of Computational Electronics, 2008, 7, 324-327.	2.5	15
97	Current-induced dynamics in carbon atomic contacts. Beilstein Journal of Nanotechnology, 2011, 2, 814-823.	2.8	15
98	Giant tunnel-electron injection in nitrogen-doped graphene. Physical Review B, 2015, 91, .	3.2	15
99	Inelastic vibrational signals in electron transport across graphene nanoconstrictions. Physical Review B, 2016, 93, .	3.2	15
100	Mechanochemistry Induced Using Force Exerted by a Functionalized Microscope Tip. Angewandte Chemie - International Edition, 2017, 56, 11769-11773.	13.8	15
101	Green function, quasi-classical Langevin and Kuboâ€“Greenwood methods in quantum thermal transport. Journal of Physics Condensed Matter, 2019, 31, 273003.	1.8	15
102	Electric-Field Control of a Single-Atom Polar Bond. Physical Review Letters, 2021, 126, 216801.	7.8	15
103	Physics of artificial nano-structures on surfaces. Progress in Surface Science, 2000, 64, 139-155.	8.3	14
104	Identification of pristine and defective graphene nanoribbons by phonon signatures in the electron transport characteristics. Physical Review B, 2015, 91, .	3.2	14
105	Modeling of Inelastic Transport in One-Dimensional Metallic Atomic Wires. Journal of Computational Electronics, 2004, 3, 423-427.	2.5	13
106	Corrections to the density-functional theory electronic spectrum: copper phthalocyanine. Applied Physics A: Materials Science and Processing, 2009, 95, 257-263.	2.3	13
107	Large-scale tight-binding simulations of quantum transport in ballistic graphene. Journal of Physics Condensed Matter, 2018, 30, 364001.	1.8	13
108	Graphene-Subgrain-Defined Oxidation of Copper. ACS Applied Materials & Interfaces, 2019, 11, 48518-48524.	8.0	13

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109	Multi-scale approach to first-principles electron transport beyond 100 nm. Nanoscale, 2019, 11, 6153-6164.	5.6	12
110	Phonon scattering in nanoscale systems: lowest order expansion of the current and power expressions. Journal of Physics: Conference Series, 2006, 35, 247-254.	0.4	11
111	Manipulating magnetism and conductance of an adatom-molecule junction on a metal surface: Anab initiostudy. Physical Review B, 2008, 78, .	3.2	11
112	Simple and efficient LCAO basis sets for the diffuse states in carbon nanostructures. Journal of Physics Condensed Matter, 2018, 30, 25LT01.	1.8	11
113	Intraconfigurational Transition due to Surface-Induced Symmetry Breaking in Noncovalently Bonded Molecules. Journal of Physical Chemistry Letters, 2020, 11, 9329-9335.	4.6	11
114	Spin-Polarizing Electron Beam Splitter from Crossed Graphene Nanoribbons. Physical Review Letters, 2022, 129, .	7.8	11
115	Phonon scattering in graphene over substrate steps. Applied Physics Letters, 2014, 105, 153108.	3.3	10
116	Simple and efficient way of speeding up transmission calculations with k-point sampling. Beilstein Journal of Nanotechnology, 2015, 6, 1603-1608.	2.8	10
117	All-graphene edge contacts: Electrical resistance of graphene T-junctions. Carbon, 2016, 101, 101-106.	10.3	10
118	Inelastic fingerprints of hydrogen contamination in atomic gold wire systems. Journal of Physics: Conference Series, 2007, 61, 312-316.	0.4	9
119	Scattering cross section of metal catalyst atoms in silicon nanowires. Physical Review B, 2010, 81, .	3.2	9
120	Current-induced atomic forces in gated graphene nanoconstrictions. Physical Review B, 2019, 100, .	3.2	9
121	Nonequilibrium Bond Forces in Single-Molecule Junctions. Nano Letters, 2019, 19, 7845-7851.	9.1	9
122	Removing all periodic boundary conditions: Efficient nonequilibrium Green's function calculations. Physical Review B, 2019, 100, .	3.2	9
123	Density functional theory calculations of quantum electron transport: carbon nanotubes-gold contacts. Advances in Quantum Chemistry, 2003, , 299-314.	0.8	8
124	Nonequilibrium electron-vibration coupling and conductance fluctuations in a C60junction. Physical Review B, 2012, 86, .	3.2	8
125	Atomistic Insight into the Formation of Metal-Graphene One-Dimensional Contacts. Physical Review Applied, 2018, 10, .	3.8	8
126	Spectroscopy of transmission resonances through a C₆₀junction. Journal of Physics Condensed Matter, 2015, 27, 015001.	1.8	7

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127	Semiconductor band alignment from first principles: A new nonequilibrium Green's function method applied to the CZTSe/CdS interface for photovoltaics. , 2016, , .		7
128	Ab initio current-induced molecular dynamics. Physical Review B, 2020, 101, .	3.2	7
129	Theory of electron transmission through atom bridges. Progress in Surface Science, 1998, 59, 245-254.	8.3	6
130	Strong spin-filtering and spin-valve effects in a molecular Vâ€“C₆₀â€“V contact. Beilstein Journal of Nanotechnology, 2012, 3, 589-596.	2.8	6
131	Local Probes of Graphene Lattice Dynamics. Small Methods, 2020, 4, 1900817.	8.6	6
132	Electrochemical Control of Charge Current Flow in Nanoporous Graphene. Advanced Functional Materials, 2021, 31, 2104031.	14.9	6
133	New Method For First Principles Modeling of Electron Transport through Nanoelectronic Devices.. Materials Research Society Symposia Proceedings, 2000, 636, 9251.	0.1	5
134	Atomic waterwheels go to work. Nature Nanotechnology, 2009, 4, 81-82.	31.5	5
135	Grain boundary-induced variability of charge transport in hydrogenated polycrystalline graphene. 2D Materials, 2017, 4, 025009.	4.4	5
136	Current-induced runaway vibrations in dehydrogenated graphene nanoribbons. Beilstein Journal of Nanotechnology, 2016, 7, 68-74.	2.8	4
137	Mechanochemistry Induced Using Force Exerted by a Functionalized Microscope Tip. Angewandte Chemie, 2017, 129, 11931-11935.	2.0	4
138	Strong paramagnon scattering in single atom Pd contacts. Physical Review B, 2017, 96, .	3.2	4
139	Control of the local magnetic states in graphene with voltage and gating. Physical Review B, 2021, 103, .	3.2	4
140	Acetylene-Mediated Electron Transport in Nanostructured Graphene and Hexagonal Boron Nitride. Journal of Physical Chemistry Letters, 2021, 12, 11220-11227.	4.6	4
141	Molecular Electronics: Insight from First-Principles Transport Simulations. Chimia, 2010, 64, 350.	0.6	3
142	Thermopower switching by magnetic field: First-principles calculations. Physical Review B, 2013, 88, .	3.2	3
143	Current shot noise in atomic contacts: Fe and FeH2 between Au electrodes. Physical Review B, 2021, 104, .	3.2	3
144	Engineering piezoresistivity using biaxially strained silicon. Applied Physics Letters, 2008, 93, 263501.	3.3	2

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145	Voltage-dependent conductance states of a single-molecule junction. Journal of Physics Condensed Matter, 2012, 24, 394012.	1.8	2
146	Comment on â€œRethinking first-principles electron transport theories with projection operators: The problems caused by partitioning the basis setâ€•[J. Chem. Phys. 139, 114104 (2013)]. Journal of Chemical Physics, 2014, 140, 177103.	3.0	2
147	Mobility and bulk electron-phonon interaction in two-dimensional materials. , 2015, , .		2
148	Tunneling spectra of graphene on copper unraveled. Physical Chemistry Chemical Physics, 2016, 18, 17081-17090.	2.8	2
149	Surface states and related quantum interference in ab initio electron transport. Physical Review Research, 2021, 3, .	3.6	2
150	Nakamuraet al.Reply:. Physical Review Letters, 2000, 84, 2549-2549.	7.8	1
151	Semiconducting IIIâ€“V nanowires with nanogaps for molecular junctions: DFT transport simulations. Nanotechnology, 2009, 20, 465401.	2.6	1
152	Ab initio vibrations in nonequilibrium nanowires. Journal of Physics: Conference Series, 2010, 220, 012010.	0.4	1
153	Directed growth of hydrogen lines on graphene: High-throughput simulations powered by evolutionary algorithm. Physical Review Materials, 2018, 2, .	2.4	1
154	DFT-NEGF Approach to Current-Induced Forces, Vibrational Signals and Heating in Nanoconductors. , 2010, , .		1
155	Proposal for All-Electrical Spin Manipulation and Detection for a Single Molecule on Boron-Substituted Graphene. Physical Review Letters, 2022, 129, .	7.8	1
156	First-principles Theory of Inelastic Transport and Local Heating in Atomic Gold Wires. AIP Conference Proceedings, 2007, , .	0.4	0
157	Thermoelectric properties of disordered graphene antidot devices. , 2012, , .		0
158	Atomistic approach for modeling metal-semiconductor interfaces. , 2016, , .		0
159	New approaches for first-principles modelling of inelastic transport in nanoscale semiconductor devices with thousands of atoms. , 2017, , .		0
160	BioFET-SIM: A Tool for the Analysis and Prediction of Signal Changes in Nanowire-Based Field Effect Transistor Biosensors. Lecture Notes in Nanoscale Science and Technology, 2013, , 55-86.	0.8	0
161	Quantum Transmission Channels in Perturbed 3D Nanowires. , 1997, , 61-78.		0
162	(Invited) First Principles Electron Transport Calculations: From Molecular Contacts to Large 2D Devices. ECS Meeting Abstracts, 2020, MA2020-01, 2769-2769.	0.0	0