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	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
2	Proposal for All-Electrical Spin Manipulation and Detection for a Single Molecule on Boron-Substituted Graphene. Physical Review Letters, 2022, 129, .	7.8	1
3	Spin-Polarizing Electron Beam Splitter from Crossed Graphene Nanoribbons. Physical Review Letters, 2022, 129, .	7.8	11
4	Electric-Field Control of a Single-Atom Polar Bond. Physical Review Letters, 2021, 126, 216801.	7.8	15
5	Control of the local magnetic states in graphene with voltage and gating. Physical Review B, 2021, 103, .	3.2	4
6	Surface states and related quantum interference in ab initio electron transport. Physical Review Research, 2021, 3, .	3.6	2
7	Electrochemical Control of Charge Current Flow in Nanoporous Graphene. Advanced Functional Materials, 2021, 31, 2104031.	14.9	6
8	Current shot noise in atomic contacts: Fe and FeH2 between Au electrodes. Physical Review B, 2021, 104, .	3.2	3
9	Acetylene-Mediated Electron Transport in Nanostructured Graphene and Hexagonal Boron Nitride. Journal of Physical Chemistry Letters, 2021, 12, 11220-11227.	4.6	4
10	QuantumATK: an integrated platform of electronic and atomic-scale modelling tools. Journal of Physics Condensed Matter, 2020, 32, 015901.	1.8	771
11	Intraconfigurational Transition due to Surface-Induced Symmetry Breaking in Noncovalently Bonded Molecules. Journal of Physical Chemistry Letters, 2020, 11, 9329-9335.	4.6	11
12	Ab initio current-induced molecular dynamics. Physical Review B, 2020, 101, .	3.2	7
13	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	3.0	229
14	Local Probes of Graphene Lattice Dynamics. Small Methods, 2020, 4, 1900817.	8.6	6
15	(Invited) First Principles Electron Transport Calculations: From Molecular Contacts to Large 2D Devices. ECS Meeting Abstracts, 2020, MA2020-01, 2769-2769.	0.0	0
16	Green function, quasi-classical Langevin and Kuboâ€“Greenwood methods in quantum thermal transport. Journal of Physics Condensed Matter, 2019, 31, 273003.	1.8	15
17	Current-induced atomic forces in gated graphene nanoconstrictions. Physical Review B, 2019, 100, .	3.2	9
18	Quantum Interference Engineering of Nanoporous Graphene for Carbon Nanocircuitry. Journal of the American Chemical Society, 2019, 141, 13081-13088.	13.7	26

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19	Nonequilibrium Bond Forces in Single-Molecule Junctions. Nano Letters, 2019, 19, 7845-7851.	9.1	9
20	Multi-scale approach to first-principles electron transport beyond 100 nm. Nanoscale, 2019, 11, 6153-6164.	5.6	12
21	Removing all periodic boundary conditions: Efficient nonequilibrium Green's function calculations. Physical Review B, 2019, 100, .	3.2	9
22	Graphene-Subgrain-Defined Oxidation of Copper. ACS Applied Materials & Interfaces, 2019, 11, 48518-48524.	8.0	13
23	Semi-classical generalized Langevin equation for equilibrium and nonequilibrium molecular dynamics simulation. Progress in Surface Science, 2019, 94, 21-40.	8.3	36
24	Electron Transport in Nanoporous Graphene: Probing the Talbot Effect. Nano Letters, 2019, 19, 576-581.	9.1	22
25	Stacked Janus Device Concepts: Abrupt pn-Junctions and Cross-Plane Channels. Nano Letters, 2018, 18, 7275-7281.	9.1	82
26	Simple and efficient LCAO basis sets for the diffuse states in carbon nanostructures. Journal of Physics Condensed Matter, 2018, 30, 25LT01.	1.8	11
27	Large-scale tight-binding simulations of quantum transport in ballistic graphene. Journal of Physics Condensed Matter, 2018, 30, 364001.	1.8	13
28	Understanding and Engineering Phonon-Mediated Tunneling into Graphene on Metal Surfaces. Nano Letters, 2018, 18, 5697-5701.	9.1	22
29	Efficient First-Principles Calculation of Phonon-Assisted Photocurrent in Large-Scale Solar-Cell Devices. Physical Review Applied, 2018, 10, .	3.8	49
30	A Graphene-Edge Ferroelectric Molecular Switch. Nano Letters, 2018, 18, 4675-4683.	9.1	21
31	Atomistic Insight into the Formation of Metal-Graphene One-Dimensional Contacts. Physical Review Applied, 2018, 10, .	3.8	8
32	Directed growth of hydrogen lines on graphene: High-throughput simulations powered by evolutionary algorithm. Physical Review Materials, 2018, 2, .	2.4	1
33	Grain boundary-induced variability of charge transport in hydrogenated polycrystalline graphene. 2D Materials, 2017, 4, 025009.	4.4	5
34	Field Effect in Graphene-Based van der Waals Heterostructures: Stacking Sequence Matters. Nano Letters, 2017, 17, 2660-2666.	9.1	21
35	Interface band gap narrowing behind open circuit voltage losses in Cu2ZnSnS4 solar cells. Applied Physics Letters, 2017, 110, .	3.3	35
36	Flexural-Phonon Scattering Induced by Electrostatic Gating in Graphene. Physical Review Letters, 2017, 118, 046601.	7.8	32

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37	A two-dimensional Dirac fermion microscope. Nature Communications, 2017, 8, 15783.	12.8	72
38	First-principles electron transport with phonon coupling: Large scale at low cost. Physical Review B, 2017, 96, .	3.2	41
39	Mechanochemistry Induced Using Force Exerted by a Functionalized Microscope Tip. Angewandte Chemie - International Edition, 2017, 56, 11769-11773.	13.8	15
40	Mechanochemistry Induced Using Force Exerted by a Functionalized Microscope Tip. Angewandte Chemie, 2017, 129, 11931-11935.	2.0	4
41	Strong paramagnon scattering in single atom Pd contacts. Physical Review B, 2017, 96, .	3.2	4
42	New approaches for first-principles modelling of inelastic transport in nanoscale semiconductor devices with thousands of atoms. , 2017, , .		0
43	Electron-phonon scattering from Green's function transport combined with molecular dynamics: Applications to mobility predictions. Physical Review B, 2017, 95, .	3.2	33
44	Improvements on non-equilibrium and transport Green function techniques: The next-generation transiesta. Computer Physics Communications, 2017, 212, 8-24.	7.5	256
45	Current-induced runaway vibrations in dehydrogenated graphene nanoribbons. Beilstein Journal of Nanotechnology, 2016, 7, 68-74.	2.8	4
46	Atomistic approach for modeling metal-semiconductor interfaces. , 2016, , .		0
47	Graphene Nanobubbles as Valley Filters and Beam Splitters. Physical Review Letters, 2016, 117, 276801.	7.8	129
48	Localized electronic states at grain boundaries on the surface of graphene and graphite. 2D Materials, 2016, 3, 031005.	4.4	26
49	Inelastic vibrational signals in electron transport across graphene nanoconstrictions. Physical Review B, 2016, 93, .	3.2	15
50	First-principles method for electron-phonon coupling and electron mobility: Applications to two-dimensional materials. Physical Review B, 2016, 93, .	3.2	216
51	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
52	Electron and phonon drag in thermoelectric transport through coherent molecular conductors. Physical Review B, 2016, 93, .	3.2	24
53	Semiconductor band alignment from first principles: A new nonequilibrium Green's function method applied to the CZTSe/CdS interface for photovoltaics. , 2016, , .		7
54	Tunneling spectra of graphene on copper unraveled. Physical Chemistry Chemical Physics, 2016, 18, 17081-17090.	2.8	2

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55	Manipulating the voltage drop in graphene nanojunctions using a gate potential. Physical Chemistry Chemical Physics, 2016, 18, 1025-1031.	2.8	39
56	All-graphene edge contacts: Electrical resistance of graphene T-junctions. Carbon, 2016, 101, 101-106.	10.3	10
57	Identification of pristine and defective graphene nanoribbons by phonon signatures in the electron transport characteristics. Physical Review B, 2015, 91, .	3.2	14
58	Giant tunnel-electron injection in nitrogen-doped graphene. Physical Review B, 2015, 91, .	3.2	15
59	Simple and efficient way of speeding up transmission calculations with k-point sampling. Beilstein Journal of Nanotechnology, 2015, 6, 1603-1608.	2.8	10
60	Unravelling the role of inelastic tunneling into pristine and defected graphene. Physical Review B, 2015, 91, .	3.2	18
61	Spectroscopy of transmission resonances through a C₆₀junction. Journal of Physics Condensed Matter, 2015, 27, 015001.	1.8	7
62	Shot Noise as a Probe of Spin-Polarized Transport through Single Atoms. Physical Review Letters, 2015, 114, 016602.	7.8	46
63	Current-Induced Forces and Hot Spots in Biased Nanojunctions. Physical Review Letters, 2015, 114, 096801.	7.8	39
64	Mobility and bulk electron-phonon interaction in two-dimensional materials. , 2015, , .		2
65	Efficient calculation of inelastic vibration signals in electron transport: Beyond the wide-band approximation. Physical Review B, 2014, 89, .	3.2	51
66	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
67	Phonon scattering in graphene over substrate steps. Applied Physics Letters, 2014, 105, 153108.	3.3	10
68	Current-induced forces: a simple derivation. European Journal of Physics, 2014, 35, 065004.	0.6	43
69	Phonon excitation and instabilities in biased graphene nanoconstrictions. Physical Review B, 2013, 88, .	3.2	18
70	Thermopower switching by magnetic field: First-principles calculations. Physical Review B, 2013, 88, .	3.2	3
71	Light emission and finite-frequency shot noise in molecular junctions: From tunneling to contact. Physical Review B, 2013, 88, .	3.2	21
72	Electronic and transport properties of kinked graphene. Beilstein Journal of Nanotechnology, 2013, 4, 103-110.	2.8	22

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73	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
74	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
75	Current-induced atomic dynamics, instabilities, and Raman signals: Quasiclassical Langevin equation approach. Physical Review B, 2012, 85, .	3.2	94
76	Light Emission Probing Quantum Shot Noise and Charge Fluctuations at a Biased Molecular Junction. Physical Review Letters, 2012, 109, 186601.	7.8	56
77	Thermoelectric properties of disordered graphene antidot devices. , 2012, , .		0
78	Nonequilibrium electron-vibration coupling and conductance fluctuations in a C60junction. Physical Review B, 2012, 86, .	3.2	8
79	Voltage-dependent conductance states of a single-molecule junction. Journal of Physics Condensed Matter, 2012, 24, 394012.	1.8	2
80	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
81	Thermoelectric properties of finite graphene antidot lattices. Physical Review B, 2011, 84, .	3.2	132
82	Quantifying signal changes in nano-wire based biosensors. Nanoscale, 2011, 3, 706-717.	5.6	37
83	Current-induced dynamics in carbon atomic contacts. Beilstein Journal of Nanotechnology, 2011, 2, 814-823.	2.8	15
84	Laserlike Vibrational Instability in Rectifying Molecular Conductors. Physical Review Letters, 2011, 107, 046801.	7.8	51
85	Ab initio vibrations in nonequilibrium nanowires. Journal of Physics: Conference Series, 2010, 220, 012010.	0.4	1
86	Localized Edge Vibrations and Edge Reconstruction by Joule Heating in Graphene Nanostructures. Physical Review Letters, 2010, 104, 036807.	7.8	34
87	Scattering cross section of metal catalyst atoms in silicon nanowires. Physical Review B, 2010, 81, .	3.2	9
88	Atomic-Scale Control of Electron Transport through Single Molecules. Physical Review Letters, 2010, 104, 176802.	7.8	74
89	Molecular Electronics: Insight from First-Principles Transport Simulations. Chimia, 2010, 64, 350.	0.6	3
90	Blowing the Fuse: Berryâ€™s Phase and Runaway Vibrations in Molecular Conductors. Nano Letters, 2010, 10, 1657-1663.	9.1	103

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91	Atomic carbon chains as spin-transmitters: An ab initio transport study. Europhysics Letters, 2010, 91, 37002.	2.0	28
92	DFT-NEGF Approach to Current-Induced Forces, Vibrational Signals and Heating in Nanoconductors. , 2010, , .		1
93	Semiconducting IIIâ€“V nanowires with nanogaps for molecular junctions: DFT transport simulations. Nanotechnology, 2009, 20, 465401.	2.6	1
94	Atomistic theory for the damping of vibrational modes in monoatomic gold chains. Physical Review B, 2009, 80, .	3.2	18
95	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
96	Corrections to the density-functional theory electronic spectrum: copper phthalocyanine. Applied Physics A: Materials Science and Processing, 2009, 95, 257-263.	2.3	13
97	Atomic waterwheels go to work. Nature Nanotechnology, 2009, 4, 81-82.	31.5	5
98	Exploring the Tilt-Angle Dependence of Electron Tunneling across Molecular Junctions of Self-Assembled Alkanethiols. ACS Nano, 2009, 3, 2073-2080.	14.6	53
99	Passing Current through Touching Molecules. Physical Review Letters, 2009, 103, 206803.	7.8	104
100	Electronic properties of graphene antidot lattices. New Journal of Physics, 2009, 11, 095020.	2.9	143
101	Density functional study of graphene antidot lattices: Roles of geometrical relaxation and spin. Physical Review B, 2009, 80, .	3.2	56
102	Electron and phonon transport in silicon nanowires: Atomistic approach to thermoelectric properties. Physical Review B, 2009, 79, .	3.2	173
103	Electronic transport properties of fullerene functionalized carbon nanotubes:Ab initioand tight-binding calculations. Physical Review B, 2009, 80, .	3.2	30
104	Conductance of Alkanedithiol Single-Molecule Junctions: A Molecular Dynamics Study. Nano Letters, 2009, 9, 117-121.	9.1	153
105	Transport in silicon nanowires: role of radial dopant profile. Journal of Computational Electronics, 2008, 7, 324-327.	2.5	15
106	Ab initiostudy of spin-dependent transport in carbon nanotubes with iron and vanadium adatoms. Physical Review B, 2008, 78, .	3.2	37
107	Unified Description of Inelastic Propensity Rules for Electron Transport through Nanoscale Junctions. Physical Review Letters, 2008, 100, 226604.	7.8	181
108	Heat Conductance Is Strongly Anisotropic for Pristine Silicon Nanowires. Nano Letters, 2008, 8, 3771-3775.	9.1	90

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109	Modeling Transport in Ultrathin Si Nanowires: Charged versus Neutral Impurities. Nano Letters, 2008, 8, 2825-2828.	9.1	34
110	Engineering piezoresistivity using biaxially strained silicon. Applied Physics Letters, 2008, 93, 263501.	3.3	2
111	Piezoresistance in p-type silicon revisited. Journal of Applied Physics, 2008, 104, .	2.5	52
112	Manipulating magnetism and conductance of an adatom-molecule junction on a metal surface: Anab initiostudy. Physical Review B, 2008, 78, .	3.2	11
113	Inelastic transport theory from first principles: Methodology and application to nanoscale devices. Physical Review B, 2007, 75, .	3.2	378
114	Screening model for nanowire surface-charge sensors in liquid. Applied Physics Letters, 2007, 91, .	3.3	39
115	Transmission eigenchannels from nonequilibrium Greenâ€™s functions. Physical Review B, 2007, 76, .	3.2	276
116	From tunneling to contact: Inelastic signals in an atomic gold junction from first principles. Physical Review B, 2007, 75, .	3.2	56
117	Inelastic fingerprints of hydrogen contamination in atomic gold wire systems. Journal of Physics: Conference Series, 2007, 61, 312-316.	0.4	9
118	Controlled Contact to aC60Molecule. Physical Review Letters, 2007, 98, 065502.	7.8	126
119	Efficient Organometallic Spin Filter between Single-Wall Carbon Nanotube or Graphene Electrodes. Physical Review Letters, 2007, 98, 197202.	7.8	133
120	Scaling Theory Put into Practice: First-Principles Modeling of Transport in Doped Silicon Nanowires. Physical Review Letters, 2007, 99, 076803.	7.8	112
121	First-principles Theory of Inelastic Transport and Local Heating in Atomic Gold Wires. AIP Conference Proceedings, 2007, , .	0.4	0
122	Ab-initio Non-Equilibrium Greenâ€™s Function Formalism for Calculating Electron Transport in Molecular Devices. , 2006, , 117-151.		16
123	Inelastic Transport through Molecules:Â Comparing First-Principles Calculations to Experiments. Nano Letters, 2006, 6, 258-262.	9.1	133
124	Organometallic Benzene-Vanadium Wire: A One-Dimensional Half-Metallic Ferromagnet. Physical Review Letters, 2006, 97, 097201.	7.8	202
125	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
126	Electronic transport through Si nanowires: Role of bulk and surface disorder. Physical Review B, 2006, 74, .	3.2	95

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127	Modeling inelastic phonon scattering in atomic- and molecular-wire junctions. Physical Review B, 2005, 72, .	3.2	192
128	Inelastic Scattering and Local Heating in Atomic Gold Wires. Physical Review Letters, 2004, 93, 256601.	7.8	204
129	Electron transport through monovalent atomic wires. Physical Review B, 2004, 69, .	3.2	125
130	Modeling of Inelastic Transport in One-Dimensional Metallic Atomic Wires. Journal of Computational Electronics, 2004, 3, 423-427.	2.5	13
131	Current-voltage relation for thin tunnel barriers: Parabolic barrier model. Journal of Applied Physics, 2004, 95, 3582-3586.	2.5	22
132	TranSIESTA: A Spice for Molecular Electronics. Annals of the New York Academy of Sciences, 2003, 1006, 212-226.	3.8	205
133	Do Aviramâ^'Ratner Diodes Rectify?. Journal of the American Chemical Society, 2003, 125, 3674-3675.	13.7	237
134	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
135	Conductance of single-atom platinum contacts: Voltage dependence of the conductance histogram. Physical Review B, 2003, 67, .	3.2	49
136	Origin of current-induced forces in an atomic gold wire:â€,â€A first-principles study. Physical Review B, 2003, 67, .	3.2	98
137	Conductance switching in a molecular device: The role of side groups and intermolecular interactions. Physical Review B, 2003, 68, .	3.2	191
138	Density functional theory calculations of quantum electron transport: carbon nanotubes-gold contacts. Advances in Quantum Chemistry, 2003, , 299-314.	0.8	8
139	Spontaneous dissociation of a conjugated molecule on the Si(100) surface. Journal of Chemical Physics, 2002, 117, 321-330.	3.0	32
140	Theory of Rectification in Tour Wires: The Role of Electrode Coupling. Physical Review Letters, 2002, 89, 138301.	7.8	327
141	Simulations of quantum transport in nanoscale systems: application to atomic gold and silver wires. Nanotechnology, 2002, 13, 346-351.	2.6	39
142	Density-functional method for nonequilibrium electron transport. Physical Review B, 2002, 65, .	3.2	4,752
143	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
144	Physics of artificial nano-structures on surfaces. Progress in Surface Science, 2000, 64, 139-155.	8.3	14

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145	New Method For First Principles Modeling of Electron Transport through Nanoelectronic Devices.. Materials Research Society Symposia Proceedings, 2000, 636, 9251.	0.1	5
146	First-principles study of electron transport through monatomic Al and Na wires. Physical Review B, 2000, 62, 8430-8437.	3.2	113
147	Current-voltage curves of gold quantum point contacts revisited. Applied Physics Letters, 2000, 77, 708-710.	3.3	82
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149	Conductance through Atoms: Dot or Channel?. Japanese Journal of Applied Physics, 1999, 38, 336-338.	1.5	35
150	Density Functional Simulation of a Breaking Nanowire. Physical Review Letters, 1999, 82, 1538-1541.	7.8	97
151	Transmission channels through Na and Al atom wire. Surface Science, 1999, 433-435, 854-857.	1.9	39
152	Conduction channels at finite bias in single-atom gold contacts. Physical Review B, 1999, 60, 17064-17070.	3.2	143
153	Mechanical deformation of atomic-scale metallic contacts: Structure and mechanisms. Physical Review B, 1998, 57, 3283-3294.	3.2	235
154	Theory of electron transmission through atom bridges. Progress in Surface Science, 1998, 59, 245-254.	8.3	6
155	Local density of states from transmission amplitudes in multichannel systems. Physical Review B, 1998, 57, R15088-R15091.	3.2	19
156	Scattering and conductance quantization in three-dimensional metal nanocontacts. Physical Review B, 1997, 55, 2637-2650.	3.2	93
157	Conductance eigenchannels in nanocontacts. Physical Review B, 1997, 56, 14956-14959.	3.2	196
158	Quantum Transmission Channels in Perturbed 3D Nanowires. , 1997, , 61-78.		0
159	Apparent Barrier Height in Scanning Tunneling Microscopy Revisited. Physical Review Letters, 1996, 76, 1485-1488.	7.8	180
160	Quantized conductance in atom-sized wires between two metals. Physical Review B, 1995, 52, 8499-8514.	3.2	307
161	Electronically driven adsorbate excitation mechanism in femtosecond-pulse laser desorption. Physical Review B, 1995, 52, 6042-6056.	3.2	199
162	Theory of the Eigler switch. Physical Review Letters, 1994, 72, 2919-2922.	7.8	35