

Mads Brandbyge

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

151 papers	12,671 citations	50 h-index	112 g-index
164 ext. papers	14,095 ext. citations	5.4 avg, IF	6.33 L-index

#	Paper	IF	Citations
151	Density-functional method for nonequilibrium electron transport. <i>Physical Review B</i> , 2002 , 65,	3.3	4039
150	Theoretical study of the nonlinear conductance of Di-thiol benzene coupled to Au(1 1 1) surfaces via thiol and thiolate bonds. <i>Computational Materials Science</i> , 2003 , 27, 151-160	3.2	425
149	Inelastic transport theory from first principles: Methodology and application to nanoscale devices. <i>Physical Review B</i> , 2007 , 75,	3.3	330
148	QuantumATK: an integrated platform of electronic and atomic-scale modelling tools. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 015901	1.8	330
147	Theory of rectification in four wires: the role of electrode coupling. <i>Physical Review Letters</i> , 2002 , 89, 138301	7.4	309
146	Quantized conductance in atom-sized wires between two metals. <i>Physical Review B</i> , 1995 , 52, 8499-8514	3.3	260
145	Transmission eigenchannels from nonequilibrium Green's functions. <i>Physical Review B</i> , 2007 , 76,	3.3	239
144	Mechanical deformation of atomic-scale metallic contacts: Structure and mechanisms. <i>Physical Review B</i> , 1998 , 57, 3283-3294	3.3	225
143	Do Aviram-Ratner diodes rectify?. <i>Journal of the American Chemical Society</i> , 2003 , 125, 3674-5	16.4	222
142	Inelastic scattering and local heating in atomic gold wires. <i>Physical Review Letters</i> , 2004 , 93, 256601	7.4	194
141	Conductance eigenchannels in nanocontacts. <i>Physical Review B</i> , 1997 , 56, 14956-14959	3.3	189
140	Organometallic benzene-vanadium wire: A one-dimensional half-metallic ferromagnet. <i>Physical Review Letters</i> , 2006 , 97, 097201	7.4	189
139	Conductance switching in a molecular device: The role of side groups and intermolecular interactions. <i>Physical Review B</i> , 2003 , 68,	3.3	187
138	Electronically driven adsorbate excitation mechanism in femtosecond-pulse laser desorption. <i>Physical Review B</i> , 1995 , 52, 6042-6056	3.3	184
137	Modeling inelastic phonon scattering in atomic- and molecular-wire junctions. <i>Physical Review B</i> , 2005 , 72,	3.3	178
136	Transiesta: a spice for molecular electronics. <i>Annals of the New York Academy of Sciences</i> , 2003 , 1006, 212-26	6.5	175
135	Unified description of inelastic propensity rules for electron transport through nanoscale junctions. <i>Physical Review Letters</i> , 2008 , 100, 226604	7.4	166

134	Improvements on non-equilibrium and transport Green function techniques: The next-generation transiesta. <i>Computer Physics Communications</i> , 2017 , 212, 8-24	4.2	155
133	Electron and phonon transport in silicon nanowires: Atomistic approach to thermoelectric properties. <i>Physical Review B</i> , 2009 , 79,	3.3	154
132	First-principles method for electron-phonon coupling and electron mobility: Applications to two-dimensional materials. <i>Physical Review B</i> , 2016 , 93,	3.3	144
131	Apparent barrier height in scanning tunneling microscopy revisited. <i>Physical Review Letters</i> , 1996 , 76, 1485-1488	7.4	142
130	Conductance of alkanedithiol single-molecule junctions: a molecular dynamics study. <i>Nano Letters</i> , 2009 , 9, 117-21	11.5	139
129	Surface-decorated silicon nanowires: a route to high-ZT thermoelectrics. <i>Physical Review Letters</i> , 2009 , 103, 055502	7.4	132
128	Conduction channels at finite bias in single-atom gold contacts. <i>Physical Review B</i> , 1999 , 60, 17064-17070,	9.3	132
127	Inelastic transport through molecules: comparing first-principles calculations to experiments. <i>Nano Letters</i> , 2006 , 6, 258-62	11.5	128
126	Efficient organometallic spin filter between single-wall carbon nanotube or graphene electrodes. <i>Physical Review Letters</i> , 2007 , 98, 197202	7.4	127
125	Controlled contact to a C60 molecule. <i>Physical Review Letters</i> , 2007 , 98, 065502	7.4	119
124	Electron transport through monovalent atomic wires. <i>Physical Review B</i> , 2004 , 69,	3.3	119
123	Electronic properties of graphene antidot lattices. <i>New Journal of Physics</i> , 2009 , 11, 095020	2.9	118
122	Thermoelectric properties of finite graphene antidot lattices. <i>Physical Review B</i> , 2011 , 84,	3.3	112
121	First-principles study of electron transport through monatomic Al and Na wires. <i>Physical Review B</i> , 2000 , 62, 8430-8437	3.3	102
120	Scaling theory put into practice: first-principles modeling of transport in doped silicon nanowires. <i>Physical Review Letters</i> , 2007 , 99, 076803	7.4	100
119	Passing current through touching molecules. <i>Physical Review Letters</i> , 2009 , 103, 206803	7.4	95
118	General atomistic approach for modeling metal-semiconductor interfaces using density functional theory and nonequilibrium Green's function. <i>Physical Review B</i> , 2016 , 93,	3.3	90
117	Density Functional Simulation of a Breaking Nanowire. <i>Physical Review Letters</i> , 1999 , 82, 1538-1541	7.4	90

116	Electronic transport through Si nanowires: Role of bulk and surface disorder. <i>Physical Review B</i> , 2006 , 74,	3.3	89
115	Current-voltage curves of atomic-sized transition metal contacts: an explanation of why Au is Ohmic and Pt is not. <i>Physical Review Letters</i> , 2002 , 89, 066804	7.4	88
114	Scattering and conductance quantization in three-dimensional metal nanocontacts. <i>Physical Review B</i> , 1997 , 55, 2637-2650	3.3	87
113	Origin of current-induced forces in an atomic gold wire: A first-principles study. <i>Physical Review B</i> , 2003 , 67,	3.3	87
112	Blowing the fuse: Berry's phase and runaway vibrations in molecular conductors. <i>Nano Letters</i> , 2010 , 10, 1657-63	11.5	86
111	Graphene Nanobubbles as Valley Filters and Beam Splitters. <i>Physical Review Letters</i> , 2016 , 117, 276801	7.4	86
110	Heat conductance is strongly anisotropic for pristine silicon nanowires. <i>Nano Letters</i> , 2008 , 8, 3771-5	11.5	82
109	Current-voltage curves of gold quantum point contacts revisited. <i>Applied Physics Letters</i> , 2000 , 77, 708-710	7.4	78
108	Current-induced atomic dynamics, instabilities, and Raman signals: Quasiclassical Langevin equation approach. <i>Physical Review B</i> , 2012 , 85,	3.3	74
107	Atomic-scale control of electron transport through single molecules. <i>Physical Review Letters</i> , 2010 , 104, 176802	7.4	71
106	Siesta: Recent developments and applications. <i>Journal of Chemical Physics</i> , 2020 , 152, 204108	3.9	69
105	From tunneling to contact: Inelastic signals in an atomic gold junction from first principles. <i>Physical Review B</i> , 2007 , 75,	3.3	55
104	Light emission probing quantum shot noise and charge fluctuations at a biased molecular junction. <i>Physical Review Letters</i> , 2012 , 109, 186601	7.4	52
103	Density functional study of graphene antidot lattices: Roles of geometrical relaxation and spin. <i>Physical Review B</i> , 2009 , 80,	3.3	52
102	A two-dimensional Dirac fermion microscope. <i>Nature Communications</i> , 2017 , 8, 15783	17.4	50
101	Exploring the tilt-angle dependence of electron tunneling across molecular junctions of self-assembled alkanethiols. <i>ACS Nano</i> , 2009 , 3, 2073-80	16.7	49
100	Conductance of single-atom platinum contacts: Voltage dependence of the conductance histogram. <i>Physical Review B</i> , 2003 , 67,	3.3	47
99	Stacked Janus Device Concepts: Abrupt pn-Junctions and Cross-Plane Channels. <i>Nano Letters</i> , 2018 , 18, 7275-7281	11.5	45

98	Laserlike vibrational instability in rectifying molecular conductors. <i>Physical Review Letters</i> , 2011 , 107, 046801	7.4	44
97	Efficient calculation of inelastic vibration signals in electron transport: Beyond the wide-band approximation. <i>Physical Review B</i> , 2014 , 89,	3.3	43
96	Piezoresistance in p-type silicon revisited. <i>Journal of Applied Physics</i> , 2008 , 104, 023715	2.5	41
95	Shot noise as a probe of spin-polarized transport through single atoms. <i>Physical Review Letters</i> , 2015 , 114, 016602	7.4	38
94	Screening model for nanowire surface-charge sensors in liquid. <i>Applied Physics Letters</i> , 2007 , 91, 102105	3.4	37
93	Ab initio study of spin-dependent transport in carbon nanotubes with iron and vanadium adatoms. <i>Physical Review B</i> , 2008 , 78,	3.3	36
92	Conductance through Atoms: Dot or Channel?. <i>Japanese Journal of Applied Physics</i> , 1999 , 38, 336-338	1.4	35
91	Transmission channels through Na and Al atom wire. <i>Surface Science</i> , 1999 , 433-435, 854-857	1.8	35
90	Simulations of quantum transport in nanoscale systems: application to atomic gold and silver wires. <i>Nanotechnology</i> , 2002 , 13, 346-351	3.4	34
89	Theory of the Eigler switch. <i>Physical Review Letters</i> , 1994 , 72, 2919-2922	7.4	34
88	Quantifying signal changes in nano-wire based biosensors. <i>Nanoscale</i> , 2011 , 3, 706-17	7.7	33
87	Localized edge vibrations and edge reconstruction by joule heating in graphene nanostructures. <i>Physical Review Letters</i> , 2010 , 104, 036807	7.4	32
86	Interface band gap narrowing behind open circuit voltage losses in Cu ₂ ZnSnS ₄ solar cells. <i>Applied Physics Letters</i> , 2017 , 110, 083903	3.4	31
85	Current-induced forces and hot spots in biased nanojunctions. <i>Physical Review Letters</i> , 2015 , 114, 096801	7.4	31
84	Modeling transport in ultrathin Si nanowires: charged versus neutral impurities. <i>Nano Letters</i> , 2008 , 8, 2825-8	11.5	31
83	Predicting and rationalizing the effect of surface charge distribution and orientation on nano-wire based FET bio-sensors. <i>Nanoscale</i> , 2011 , 3, 3635-40	7.7	28
82	Electronic transport properties of fullerene functionalized carbon nanotubes: Ab initio and tight-binding calculations. <i>Physical Review B</i> , 2009 , 80,	3.3	27
81	Efficient First-Principles Calculation of Phonon-Assisted Photocurrent in Large-Scale Solar-Cell Devices. <i>Physical Review Applied</i> , 2018 , 10,	4.3	26

80	Atomic carbon chains as spin-transmitters: An ab initio transport study. <i>Europhysics Letters</i> , 2010 , 91, 37002	1.6	26
79	Localized electronic states at grain boundaries on the surface of graphene and graphite. <i>2D Materials</i> , 2016 , 3, 031005	5.9	26
78	Spontaneous dissociation of a conjugated molecule on the Si(100) surface. <i>Journal of Chemical Physics</i> , 2002 , 117, 321-330	3.9	25
77	Manipulating the voltage drop in graphene nanojunctions using a gate potential. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 1025-31	3.6	24
76	Flexural-Phonon Scattering Induced by Electrostatic Gating in Graphene. <i>Physical Review Letters</i> , 2017 , 118, 046601	7.4	23
75	Electron-phonon scattering from Green's function transport combined with molecular dynamics: Applications to mobility predictions. <i>Physical Review B</i> , 2017 , 95,	3.3	22
74	Semi-classical generalized Langevin equation for equilibrium and nonequilibrium molecular dynamics simulation. <i>Progress in Surface Science</i> , 2019 , 94, 21-40	6.6	21
73	Current-induced forces: a simple derivation. <i>European Journal of Physics</i> , 2014 , 35, 065004	0.8	20
72	First-principles electron transport with phonon coupling: Large scale at low cost. <i>Physical Review B</i> , 2017 , 96,	3.3	19
71	Electron and phonon drag in thermoelectric transport through coherent molecular conductors. <i>Physical Review B</i> , 2016 , 93,	3.3	19
70	Electronic and transport properties of kinked graphene. <i>Beilstein Journal of Nanotechnology</i> , 2013 , 4, 103-10	3	19
69	Current-voltage relation for thin tunnel barriers: Parabolic barrier model. <i>Journal of Applied Physics</i> , 2004 , 95, 3582-3586	2.5	19
68	Understanding and Engineering Phonon-Mediated Tunneling into Graphene on Metal Surfaces. <i>Nano Letters</i> , 2018 , 18, 5697-5701	11.5	18
67	Quantum Interference Engineering of Nanoporous Graphene for Carbon Nanocircuitry. <i>Journal of the American Chemical Society</i> , 2019 , 141, 13081-13088	16.4	17
66	Phonon excitation and instabilities in biased graphene nanoconstrictions. <i>Physical Review B</i> , 2013 , 88,	3.3	17
65	Unravelling the role of inelastic tunneling into pristine and defected graphene. <i>Physical Review B</i> , 2015 , 91,	3.3	17
64	Light emission and finite-frequency shot noise in molecular junctions: From tunneling to contact. <i>Physical Review B</i> , 2013 , 88,	3.3	17
63	Atomistic theory for the damping of vibrational modes in monoatomic gold chains. <i>Physical Review B</i> , 2009 , 80,	3.3	17

62	Local density of states from transmission amplitudes in multichannel systems. <i>Physical Review B</i> , 1998 , 57, R15088-R15091	3.3	17
61	A Graphene-Edge Ferroelectric Molecular Switch. <i>Nano Letters</i> , 2018 , 18, 4675-4683	11.5	15
60	Transport in silicon nanowires: role of radial dopant profile. <i>Journal of Computational Electronics</i> , 2008 , 7, 324-327	1.8	15
59	Electron Transport in Nanoporous Graphene: Probing the Talbot Effect. <i>Nano Letters</i> , 2019 , 19, 576-581	11.5	15
58	Field Effect in Graphene-Based van der Waals Heterostructures: Stacking Sequence Matters. <i>Nano Letters</i> , 2017 , 17, 2660-2666	11.5	14
57	Current-induced dynamics in carbon atomic contacts. <i>Beilstein Journal of Nanotechnology</i> , 2011 , 2, 814-23		14
56	Mechanochemistry Induced Using Force Exerted by a Functionalized Microscope Tip. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 11769-11773	16.4	13
55	Modeling of Inelastic Transport in One-Dimensional Metallic Atomic Wires. <i>Journal of Computational Electronics</i> , 2004 , 3, 423-427	1.8	13
54	Ab-initio Non-Equilibrium Green's Function Formalism for Calculating Electron Transport in Molecular Devices 2006 , 117-151		12
53	Physics of artificial nano-structures on surfaces. <i>Progress in Surface Science</i> , 2000 , 64, 139-155	6.6	12
52	Inelastic vibrational signals in electron transport across graphene nanoconstrictions. <i>Physical Review B</i> , 2016 , 93,	3.3	11
51	Identification of pristine and defective graphene nanoribbons by phonon signatures in the electron transport characteristics. <i>Physical Review B</i> , 2015 , 91,	3.3	11
50	Giant tunnel-electron injection in nitrogen-doped graphene. <i>Physical Review B</i> , 2015 , 91,	3.3	11
49	Corrections to the density-functional theory electronic spectrum: copper phthalocyanine. <i>Applied Physics A: Materials Science and Processing</i> , 2009 , 95, 257-263	2.6	11
48	Manipulating magnetism and conductance of an adatom-molecule junction on a metal surface: An ab initio study. <i>Physical Review B</i> , 2008 , 78,	3.3	11
47	Simple and efficient way of speeding up transmission calculations with k-point sampling. <i>Beilstein Journal of Nanotechnology</i> , 2015 , 6, 1603-8	3	10
46	Phonon scattering in graphene over substrate steps. <i>Applied Physics Letters</i> , 2014 , 105, 153108	3.4	10
45	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	10

44	Green function, quasi-classical Langevin and Kubo-Greenwood methods in quantum thermal transport. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 273003	1.8	9
43	Inelastic fingerprints of hydrogen contamination in atomic gold wire systems. <i>Journal of Physics: Conference Series</i> , 2007 , 61, 312-316	0.3	9
42	Simple and efficient LCAO basis sets for the diffuse states in carbon nanostructures. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 25LT01	1.8	9
41	Multi-scale approach to first-principles electron transport beyond 100 nm. <i>Nanoscale</i> , 2019 , 11, 6153-6164	1.7	8
40	Nonequilibrium electron-vibration coupling and conductance fluctuations in a C60 junction. <i>Physical Review B</i> , 2012 , 86,	3.3	8
39	Scattering cross section of metal catalyst atoms in silicon nanowires. <i>Physical Review B</i> , 2010 , 81,	3.3	8
38	Graphene-Subgrain-Defined Oxidation of Copper. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 48518-48524	1.5	8
37	All-graphene edge contacts: Electrical resistance of graphene T-junctions. <i>Carbon</i> , 2016 , 101, 101-106	10.4	7
36	Large-scale tight-binding simulations of quantum transport in ballistic graphene. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 364001	1.8	7
35	Spectroscopy of transmission resonances through a C ₆₀ junction. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 015001	1.8	7
34	Atomistic Insight into the Formation of Metal-Graphene One-Dimensional Contacts. <i>Physical Review Applied</i> , 2018 , 10,	4.3	6
33	Current-induced atomic forces in gated graphene nanoconstrictions. <i>Physical Review B</i> , 2019 , 100,	3.3	6
32	Strong spin-filtering and spin-valve effects in a molecular V-C(60)-V contact. <i>Beilstein Journal of Nanotechnology</i> , 2012 , 3, 589-96	3	6
31	Theory of electron transmission through atom bridges. <i>Progress in Surface Science</i> , 1998 , 59, 245-254	6.6	6
30	Density functional theory calculations of quantum electron transport: carbon nanotubes-gold contacts. <i>Advances in Quantum Chemistry</i> , 2003 , 299-314	1.4	5
29	Grain boundary-induced variability of charge transport in hydrogenated polycrystalline graphene. <i>2D Materials</i> , 2017 , 4, 025009	5.9	4
28	Nonequilibrium Bond Forces in Single-Molecule Junctions. <i>Nano Letters</i> , 2019 , 19, 7845-7851	11.5	4
27	Local Probes of Graphene Lattice Dynamics. <i>Small Methods</i> , 2020 , 4, 1900817	12.8	4

26	Removing all periodic boundary conditions: Efficient nonequilibrium Green's function calculations. <i>Physical Review B</i> , 2019 , 100,	3.3	4
25	Ab initio current-induced molecular dynamics. <i>Physical Review B</i> , 2020 , 101,	3.3	3
24	Semiconductor band alignment from first principles: A new nonequilibrium Green's function method applied to the CZTSe/CdS interface for photovoltaics 2016 ,		3
23	Mechanochemistry Induced Using Force Exerted by a Functionalized Microscope Tip. <i>Angewandte Chemie</i> , 2017 , 129, 11931-11935	3.6	3
22	Thermopower switching by magnetic field: First-principles calculations. <i>Physical Review B</i> , 2013 , 88,	3.3	3
21	Molecular electronics: insight from first-principles transport simulations. <i>Chimia</i> , 2010 , 64, 350-5	1.3	3
20	Electric-Field Control of a Single-Atom Polar Bond. <i>Physical Review Letters</i> , 2021 , 126, 216801	7.4	3
19	Mobility and bulk electron-phonon interaction in two-dimensional materials 2015 ,		2
18	Tunneling spectra of graphene on copper unraveled. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 17081-90	3.9	2
17	Comment on "Rethinking first-principles electron transport theories with projection operators: the problems caused by partitioning the basis set" [J. Chem. Phys. 139, 114104 (2013)]. <i>Journal of Chemical Physics</i> , 2014 , 140, 177103	3.9	2
16	Intraconfigurational Transition due to Surface-Induced Symmetry Breaking in Noncovalently Bonded Molecules. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 9329-9335	6.4	2
15	Current-induced runaway vibrations in dehydrogenated graphene nanoribbons. <i>Beilstein Journal of Nanotechnology</i> , 2016 , 7, 68-74	3	2
14	Current shot noise in atomic contacts: Fe and FeH ₂ between Au electrodes. <i>Physical Review B</i> , 2021 , 104,	3.3	2
13	Strong paramagnon scattering in single atom Pd contacts. <i>Physical Review B</i> , 2017 , 96,	3.3	1
12	Voltage-dependent conductance states of a single-molecule junction. <i>Journal of Physics Condensed Matter</i> , 2012 , 24, 394012	1.8	1
11	Semiconducting III-V nanowires with nanogaps for molecular junctions: DFT transport simulations. <i>Nanotechnology</i> , 2009 , 20, 465401	3.4	1
10	Ab initio vibrations in nonequilibrium nanowires. <i>Journal of Physics: Conference Series</i> , 2010 , 220, 012010	0.3	1
9	Engineering piezoresistivity using biaxially strained silicon. <i>Applied Physics Letters</i> , 2008 , 93, 263501	3.4	1

8	New Method For First Principles Modeling of Electron Transport through Nanoelectronic Devices. <i>Materials Research Society Symposia Proceedings</i> , 2000 , 636, 9251		1
7	Directed growth of hydrogen lines on graphene: High-throughput simulations powered by evolutionary algorithm. <i>Physical Review Materials</i> , 2018 , 2,	3.2	1
6	DFT-NEGF Approach to Current-Induced Forces, Vibrational Signals and Heating in Nanoconductors 2010 ,		1
5	Electrochemical Control of Charge Current Flow in Nanoporous Graphene. <i>Advanced Functional Materials</i> , 2021 , 31, 2104031	15.6	1
4	Acetylene-Mediated Electron Transport in Nanostructured Graphene and Hexagonal Boron Nitride. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 11220-11227	6.4	0
3	Nakamura et al. reply:. <i>Physical Review Letters</i> , 2000 , 84, 2549	7.4	
2	Quantum Transmission Channels in Perturbed 3D Nanowires 1997 , 61-78		
1	BioFET-SIM: A Tool for the Analysis and Prediction of Signal Changes in Nanowire-Based Field Effect Transistor Biosensors. <i>Lecture Notes in Nanoscale Science and Technology</i> , 2013 , 55-86	0.3	