Mads Brandbyge

List of Publications by Year in Descending Order

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	Acetylene-Mediated Electron Transport in Nanostructured Graphene and Hexagonal Boron Nitride. *Journal of Physical Chemistry Letters*, **2021**, 12, 11220-11227	6.4	0
150	Electric-Field Control of a Single-Atom Polar Bond. *Physical Review Letters*, **2021**, 126, 216801	7.4	3
149	Electrochemical Control of Charge Current Flow in Nanoporous Graphene. *Advanced Functional Materials*, **2021**, 31, 2104031	15.6	1
148	Current shot noise in atomic contacts: Fe and FeH2 between Au electrodes. *Physical Review B*, **2021** , 104,	3.3	2
147	Ab initio current-induced molecular dynamics. *Physical Review B*, **2020**, 101,	3.3	3
146	Siesta: Recent developments and applications. *Journal of Chemical Physics*, **2020**, 152, 204108	3.9	69
145	Local Probes of Graphene Lattice Dynamics. *Small Methods*, **2020**, 4, 1900817	12.8	4
144	QuantumATK: an integrated platform of electronic and atomic-scale modelling tools. *Journal of Physics Condensed Matter*, **2020**, 32, 015901	1.8	330
143	Intraconfigurational Transition due to Surface-Induced Symmetry Breaking in Noncovalently Bonded Molecules. *Journal of Physical Chemistry Letters*, **2020**, 11, 9329-9335	6.4	2
142	Nonequilibrium Bond Forces in Single-Molecule Junctions. *Nano Letters*, **2019**, 19, 7845-7851	11.5	4
141	Multi-scale approach to first-principles electron transport beyond 100 nm. *Nanoscale*, **2019**, 11, 6153-6164	7.7	8
140	Green function, quasi-classical Langevin and Kubo-Greenwood methods in quantum thermal transport. *Journal of Physics Condensed Matter*, **2019**, 31, 273003	1.8	9
139	Current-induced atomic forces in gated graphene nanoconstrictions. *Physical Review B*, **2019**, 100,	3.3	6
138	Quantum Interference Engineering of Nanoporous Graphene for Carbon Nanocircuitry. *Journal of the American Chemical Society*, **2019**, 141, 13081-13088	16.4	17
137	Removing all periodic boundary conditions: Efficient nonequilibrium Green's function calculations. *Physical Review B*, **2019**, 100,	3.3	4
136	Graphene-Subgrain-Defined Oxidation of Copper. *ACS Applied Materials & Interfaces*, **2019**, 11, 48518-48524	9.5	21
135	Semi-classical generalized Langevin equation for equilibrium and nonequilibrium molecular dynamics simulation. *Progress in Surface Science*, **2019**, 94, 21-40	6.6	21

134	Electron Transport in Nanoporous Graphene: Probing the Talbot Effect. *Nano Letters*, **2019**, 19, 576-581	11.5	15
133	Large-scale tight-binding simulations of quantum transport in ballistic graphene. *Journal of Physics Condensed Matter*, **2018**, 30, 364001	1.8	7
132	Understanding and Engineering Phonon-Mediated Tunneling into Graphene on Metal Surfaces. *Nano Letters*, **2018**, 18, 5697-5701	11.5	18
131	Efficient First-Principles Calculation of Phonon-Assisted Photocurrent in Large-Scale Solar-Cell Devices. *Physical Review Applied*, **2018**, 10,	4.3	26
130	A Graphene-Edge Ferroelectric Molecular Switch. *Nano Letters*, **2018**, 18, 4675-4683	11.5	15
129	Atomistic Insight into the Formation of Metal-Graphene One-Dimensional Contacts. *Physical Review Applied*, **2018**, 10,	4.3	6
128	Directed growth of hydrogen lines on graphene: High-throughput simulations powered by evolutionary algorithm. *Physical Review Materials*, **2018**, 2,	3.2	1
127	Stacked Janus Device Concepts: Abrupt pn-Junctions and Cross-Plane Channels. *Nano Letters*, **2018**, 18, 7275-7281	11.5	45
126	Simple and efficient LCAO basis sets for the diffuse states in carbon nanostructures. *Journal of Physics Condensed Matter*, **2018**, 30, 25LT01	1.8	9
125	Grain boundary-induced variability of charge transport in hydrogenated polycrystalline graphene. *2D Materials*, **2017**, 4, 025009	5.9	4
124	Field Effect in Graphene-Based van der Waals Heterostructures: Stacking Sequence Matters. *Nano Letters*, **2017**, 17, 2660-2666	11.5	14
123	Interface band gap narrowing behind open circuit voltage losses in Cu2ZnSnS4 solar cells. *Applied Physics Letters*, **2017**, 110, 083903	3.4	31
122	Flexural-Phonon Scattering Induced by Electrostatic Gating in Graphene. *Physical Review Letters*, **2017**, 118, 046601	7.4	23
121	A two-dimensional Dirac fermion microscope. *Nature Communications*, **2017**, 8, 15783	17.4	50
120	First-principles electron transport with phonon coupling: Large scale at low cost. *Physical Review B*, **2017**, 96,	3.3	19
119	Mechanochemistry Induced Using Force Exerted by a Functionalized Microscope Tip. *Angewandte Chemie - International Edition*, **2017**, 56, 11769-11773	16.4	13
118	Mechanochemistry Induced Using Force Exerted by a Functionalized Microscope Tip. *Angewandte Chemie*, **2017**, 129, 11931-11935	3.6	3
117	Strong paramagnon scattering in single atom Pd contacts. *Physical Review B*, **2017**, 96,	3.3	1

116	Electron-phonon scattering from Green's function transport combined with molecular dynamics: Applications to mobility predictions. *Physical Review B*, **2017**, 95,	3.3	22
115	Improvements on non-equilibrium and transport Green function techniques: The next-generation transiesta. *Computer Physics Communications*, **2017**, 212, 8-24	4.2	155
114	Inelastic vibrational signals in electron transport across graphene nanoconstrictions. *Physical Review B*, **2016**, 93,	3.3	11
113	First-principles method for electron-phonon coupling and electron mobility: Applications to two-dimensional materials. *Physical Review B*, **2016**, 93,	3.3	144
112	General atomistic approach for modeling metal-semiconductor interfaces using density functional theory and nonequilibrium Green's function. *Physical Review B*, **2016**, 93,	3.3	90
111	Electron and phonon drag in thermoelectric transport through coherent molecular conductors. *Physical Review B*, **2016**, 93,	3.3	19
110	Semiconductor band alignment from first principles: A new nonequilibrium Green's function method applied to the CZTSe/CdS interface for photovoltaics **2016**,		3
109	Tunneling spectra of graphene on copper unraveled. *Physical Chemistry Chemical Physics*, **2016**, 18, 17081-90	3.6	2
108	Manipulating the voltage drop in graphene nanojunctions using a gate potential. *Physical Chemistry Chemical Physics*, **2016**, 18, 1025-31	3.6	24
107	All-graphene edge contacts: Electrical resistance of graphene T-junctions. *Carbon*, **2016**, 101, 101-106	10.4	7
106	Current-induced runaway vibrations in dehydrogenated graphene nanoribbons. *Beilstein Journal of Nanotechnology*, **2016**, 7, 68-74	3	2
105	Graphene Nanobubbles as Valley Filters and Beam Splitters. *Physical Review Letters*, **2016**, 117, 276801	7.4	86
104	Localized electronic states at grain boundaries on the surface of graphene and graphite. *2D Materials*, **2016**, 3, 031005	5.9	26
103	Current-induced forces and hot spots in biased nanojunctions. *Physical Review Letters*, **2015**, 114, 096801	7.4	31
102	Mobility and bulk electron-phonon interaction in two-dimensional materials **2015**,		2
101	Identification of pristine and defective graphene nanoribbons by phonon signatures in the electron transport characteristics. *Physical Review B*, **2015**, 91,	3.3	11
100	Giant tunnel-electron injection in nitrogen-doped graphene. *Physical Review B*, **2015**, 91,	3.3	11
99	Simple and efficient way of speeding up transmission calculations with k-point sampling. *Beilstein Journal of Nanotechnology*, **2015**, 6, 1603-8	3	10

98	Unravelling the role of inelastic tunneling into pristine and defected graphene. *Physical Review B*, **2015**, 91,	3.3	17
97	Spectroscopy of transmission resonances through a C□junction. *Journal of Physics Condensed Matter*, **2015**, 27, 015001	1.8	7
96	Shot noise as a probe of spin-polarized transport through single atoms. *Physical Review Letters*, **2015**, 114, 016602	7.4	38
95	Current-induced forces: a simple derivation. *European Journal of Physics*, **2014**, 35, 065004	0.8	20
94	Efficient calculation of inelastic vibration signals in electron transport: Beyond the wide-band approximation. *Physical Review B*, **2014**, 89,	3.3	43
93	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)]. *Journal of Chemical Physics*, **2014**, 140, 177103	3.9	2
92	Phonon scattering in graphene over substrate steps. *Applied Physics Letters*, **2014**, 105, 153108	3.4	10
91	Phonon excitation and instabilities in biased graphene nanoconstrictions. *Physical Review B*, **2013**, 88,	3.3	17
90	Thermopower switching by magnetic field: First-principles calculations. *Physical Review B*, **2013**, 88,	3.3	3
89	Light emission and finite-frequency shot noise in molecular junctions: From tunneling to contact. *Physical Review B*, **2013**, 88,	3.3	17
88	Electronic and transport properties of kinked graphene. *Beilstein Journal of Nanotechnology*, **2013**, 4, 103-10	3	19
87	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	0.3	
86	Nonequilibrium electron-vibration coupling and conductance fluctuations in a C60 junction. *Physical Review B*, **2012**, 86,	3.3	8
85	Voltage-dependent conductance states of a single-molecule junction. *Journal of Physics Condensed Matter*, **2012**, 24, 394012	1.8	1
84	Strong spin-filtering and spin-valve effects in a molecular V-C(60)-V contact. *Beilstein Journal of Nanotechnology*, **2012**, 3, 589-96	3	6
83	Current-induced atomic dynamics, instabilities, and Raman signals: Quasiclassical Langevin equation approach. *Physical Review B*, **2012**, 85,	3.3	74
82	Light emission probing quantum shot noise and charge fluctuations at a biased molecular junction. *Physical Review Letters*, **2012**, 109, 186601	7.4	52
81	Predicting and rationalizing the effect of surface charge distribution and orientation on nano-wire based FET bio-sensors. *Nanoscale*, **2011**, 3, 3635-40	7.7	28

80	Thermoelectric properties of finite graphene antidot lattices. *Physical Review B*, **2011**, 84,	3.3	112
79	Quantifying signal changes in nano-wire based biosensors. *Nanoscale*, **2011**, 3, 706-17	7.7	33
78	Current-induced dynamics in carbon atomic contacts. *Beilstein Journal of Nanotechnology*, **2011**, 2, 814-23	3	14
77	Laserlike vibrational instability in rectifying molecular conductors. *Physical Review Letters*, **2011**, 107, 046801	7.4	44
76	Localized edge vibrations and edge reconstruction by joule heating in graphene nanostructures. *Physical Review Letters*, **2010**, 104, 036807	7.4	32
75	Scattering cross section of metal catalyst atoms in silicon nanowires. *Physical Review B*, **2010**, 81,	3.3	8
74	Atomic-scale control of electron transport through single molecules. *Physical Review Letters*, **2010**, 104, 176802	7.4	71
73	Molecular electronics: insight from first-principles transport simulations. *Chimia*, **2010**, 64, 350-5	1.3	3
72	Blowing the fuse: Berry's phase and runaway vibrations in molecular conductors. *Nano Letters*, **2010**, 10, 1657-63	11.5	86
71	Atomic carbon chains as spin-transmitters: An ab initio transport study. *Europhysics Letters*, **2010**, 91, 37002	1.6	26
70	Ab initio vibrations in nonequilibrium nanowires. *Journal of Physics: Conference Series*, **2010**, 220, 012010	0.3	1
69	DFT-NEGF Approach to Current-Induced Forces, Vibrational Signals and Heating in Nanoconductors **2010**,		1
68	Semiconducting III-V nanowires with nanogaps for molecular junctions: DFT transport simulations. *Nanotechnology*, **2009**, 20, 465401	3.4	1
67	Atomistic theory for the damping of vibrational modes in monoatomic gold chains. *Physical Review B*, **2009**, 80,	3.3	17
66	Surface-decorated silicon nanowires: a route to high-ZT thermoelectrics. *Physical Review Letters*, **2009**, 103, 055502	7.4	132
65	Corrections to the density-functional theory electronic spectrum: copper phthalocyanine. *Applied Physics A: Materials Science and Processing*, **2009**, 95, 257-263	2.6	11
64	Exploring the tilt-angle dependence of electron tunneling across molecular junctions of self-assembled alkanethiols. *ACS Nano*, **2009**, 3, 2073-80	16.7	49
63	Passing current through touching molecules. *Physical Review Letters*, **2009**, 103, 206803	7.4	95

62	Electronic properties of graphene antidot lattices. *New Journal of Physics*, **2009**, 11, 095020	2.9	118
61	Density functional study of graphene antidot lattices: Roles of geometrical relaxation and spin. *Physical Review B*, **2009**, 80,	3.3	52
60	Electron and phonon transport in silicon nanowires: Atomistic approach to thermoelectric properties. *Physical Review B*, **2009**, 79,	3.3	154
59	Electronic transport properties of fullerene functionalized carbon nanotubes: Ab initio and tight-binding calculations. *Physical Review B*, **2009**, 80,	3.3	27
58	Conductance of alkanedithiol single-molecule junctions: a molecular dynamics study. *Nano Letters*, **2009**, 9, 117-21	11.5	139
57	Ab initio study of spin-dependent transport in carbon nanotubes with iron and vanadium adatoms. *Physical Review B*, **2008**, 78,	3.3	36
56	Unified description of inelastic propensity rules for electron transport through nanoscale junctions. *Physical Review Letters*, **2008**, 100, 226604	7.4	166
55	Heat conductance is strongly anisotropic for pristine silicon nanowires. *Nano Letters*, **2008**, 8, 3771-5	11.5	82
54	Modeling transport in ultrathin Si nanowires: charged versus neutral impurities. *Nano Letters*, **2008**, 8, 2825-8	11.5	31
53	Engineering piezoresistivity using biaxially strained silicon. *Applied Physics Letters*, **2008**, 93, 263501	3.4	1
52	Piezoresistance in p-type silicon revisited. *Journal of Applied Physics*, **2008**, 104, 023715	2.5	41
51	Manipulating magnetism and conductance of an adatom-molecule junction on a metal surface: An ab initio study. *Physical Review B*, **2008**, 78,	3.3	11
50	Transport in silicon nanowires: role of radial dopant profile. *Journal of Computational Electronics*, **2008**, 7, 324-327	1.8	15
49	Controlled contact to a C60 molecule. *Physical Review Letters*, **2007**, 98, 065502	7.4	119
48	Efficient organometallic spin filter between single-wall carbon nanotube or graphene electrodes. *Physical Review Letters*, **2007**, 98, 197202	7.4	127
47	Scaling theory put into practice: first-principles modeling of transport in doped silicon nanowires. *Physical Review Letters*, **2007**, 99, 076803	7.4	100
46	Inelastic transport theory from first principles: Methodology and application to nanoscale devices. *Physical Review B*, **2007**, 75,	3.3	330
45	Screening model for nanowire surface-charge sensors in liquid. *Applied Physics Letters*, **2007**, 91, 102105	3.4	37

44	Transmission eigenchannels from nonequilibrium Green functions. *Physical Review B*, **2007**, 76,	3.3	239
43	From tunneling to contact: Inelastic signals in an atomic gold junction from first principles. *Physical Review B*, **2007**, 75,	3.3	55
42	Inelastic fingerprints of hydrogen contamination in atomic gold wire systems. *Journal of Physics: Conference Series*, **2007**, 61, 312-316	0.3	9
41	Electronic transport through Si nanowires: Role of bulk and surface disorder. *Physical Review B*, **2006**, 74,	3.3	89
40	Ab-initio Non-Equilibrium Green Function Formalism for Calculating Electron Transport in Molecular Devices **2006**, 117-151		12
39	Inelastic transport through molecules: comparing first-principles calculations to experiments. *Nano Letters*, **2006**, 6, 258-62	11.5	128
38	Organometallic benzene-vanadium wire: A one-dimensional half-metallic ferromagnet. *Physical Review Letters*, **2006**, 97, 097201	7.4	189
37	Phonon scattering in nanoscale systems: lowest order expansion of the current and power expressions. *Journal of Physics: Conference Series*, **2006**, 35, 247-254	0.3	10
36	Modeling inelastic phonon scattering in atomic- and molecular-wire junctions. *Physical Review B*, **2005**, 72,	3.3	178
35	Inelastic scattering and local heating in atomic gold wires. *Physical Review Letters*, **2004**, 93, 256601	7.4	194
34	Electron transport through monovalent atomic wires. *Physical Review B*, **2004**, 69,	3.3	119
33	Modeling of Inelastic Transport in One-Dimensional Metallic Atomic Wires. *Journal of Computational Electronics*, **2004**, 3, 423-427	1.8	13
32	Current-voltage relation for thin tunnel barriers: Parabolic barrier model. *Journal of Applied Physics*, **2004**, 95, 3582-3586	2.5	19
31	Density functional theory calculations of quantum electron transport: carbon nanotubes-gold contacts. *Advances in Quantum Chemistry*, **2003**, 299-314	1.4	5
30	TranSIESTA: a spice for molecular electronics. *Annals of the New York Academy of Sciences*, **2003**, 1006, 212-26	6.5	175
29	Do Aviram-Ratner diodes rectify?. *Journal of the American Chemical Society*, **2003**, 125, 3674-5	16.4	222
28	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	3.2	425
27	Conductance of single-atom platinum contacts: Voltage dependence of the conductance histogram. *Physical Review B*, **2003**, 67,	3.3	47

26	Origin of current-induced forces in an atomic gold wire: A first-principles study. *Physical Review B*, **2003**, 67,	3.3	87
25	Conductance switching in a molecular device: The role of side groups and intermolecular interactions. *Physical Review B*, **2003**, 68,	3.3	187
24	Spontaneous dissociation of a conjugated molecule on the Si(100) surface. *Journal of Chemical Physics*, **2002**, 117, 321-330	3.9	25
23	Theory of rectification in tour wires: the role of electrode coupling. *Physical Review Letters*, **2002**, 89, 138301	7.4	309
22	Simulations of quantum transport in nanoscale systems: application to atomic gold and silver wires. *Nanotechnology*, **2002**, 13, 346-351	3.4	34
21	Density-functional method for nonequilibrium electron transport. *Physical Review B*, **2002**, 65,	3.3	4039
20	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	7.4	88
19	Physics of artificial nano-structures on surfaces. *Progress in Surface Science*, **2000**, 64, 139-155	6.6	12
18	New Method For First Principles Modeling of Electron Transport through Nanoelectronic Devices. *Materials Research Society Symposia Proceedings*, **2000**, 636, 9251		1
17	First-principles study of electron transport through monatomic Al and Na wires. *Physical Review B*, **2000**, 62, 8430-8437	3.3	102
16	Current-voltage curves of gold quantum point contacts revisited. *Applied Physics Letters*, **2000**, 77, 708-710	3.4	78
15	Nakamura et al. reply:. *Physical Review Letters*, **2000**, 84, 2549	7.4	
14	Conductance through Atoms: Dot or Channel?. *Japanese Journal of Applied Physics*, **1999**, 38, 336-338	1.4	35
13	Density Functional Simulation of a Breaking Nanowire. *Physical Review Letters*, **1999**, 82, 1538-1541	7.4	90
12	Transmission channels through Na and Al atom wire. *Surface Science*, **1999**, 433-435, 854-857	1.8	35
11	Conduction channels at finite bias in single-atom gold contacts. *Physical Review B*, **1999**, 60, 17064-17070	3.3	132
10	Mechanical deformation of atomic-scale metallic contacts: Structure and mechanisms. *Physical Review B*, **1998**, 57, 3283-3294	3.3	225
9	Theory of electron transmission through atom bridges. *Progress in Surface Science*, **1998**, 59, 245-254	6.6	6

8	Local density of states from transmission amplitudes in multichannel systems. *Physical Review B*, **1998**, 57, R15088-R15091	3.3	17
7	Scattering and conductance quantization in three-dimensional metal nanocontacts. *Physical Review B*, **1997**, 55, 2637-2650	3.3	87
6	Conductance eigenchannels in nanocontacts. *Physical Review B*, **1997**, 56, 14956-14959	3.3	189
5	Quantum Transmission Channels in Perturbed 3D Nanowires **1997**, 61-78		
4	Apparent barrier height in scanning tunneling microscopy revisited. *Physical Review Letters*, **1996**, 76, 1485-1488	7.4	142
3	Quantized conductance in atom-sized wires between two metals. *Physical Review B*, **1995**, 52, 8499-8514	3.3	260
2	Electronically driven adsorbate excitation mechanism in femtosecond-pulse laser desorption. *Physical Review B*, **1995**, 52, 6042-6056	3.3	184
1	Theory of the Eigler switch. *Physical Review Letters*, **1994**, 72, 2919-2922	7.4	34