Troels Markussen

List of Publications by Year
in descending order

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56	3,847	172457	233421
papers	citations	29 h-index	45 g-index

56	56	56	3812
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electron-Induced Spin-Crossover in Self-Assembled Tetramers. ACS Nano, 2021, 15, 11770-11778.	14.6	10
2	QuantumATK: an integrated platform of electronic and atomic-scale modelling tools. Journal of Physics Condensed Matter, 2020, 32, 015901.	1.8	771
3	First-Principles Evaluation of fcc Ruthenium for its use in Advanced Interconnects. Physical Review Applied, 2020, 13, .	3.8	12
4	First-Principles Quantum Transport Modeling of Spin-Transfer and Spin-Orbit Torques in Magnetic Multilayers. , 2020, , 499-533.		2
5	Grain boundary scattering in Ru and Cu interconnects. , 2020, , .		1
6	First-Principles Quantum Transport Modeling of Spin-Transfer and Spin-Orbit Torques in Magnetic Multilayers. , 2018, , 1-35.		6
7	Stacked Janus Device Concepts: Abrupt pn-Junctions and Cross-Plane Channels. Nano Letters, 2018, 18, 7275-7281.	9.1	82
8	Efficient First-Principles Calculation of Phonon-Assisted Photocurrent in Large-Scale Solar-Cell Devices. Physical Review Applied, 2018, 10, .	3.8	49
9	Interface band gap narrowing behind open circuit voltage losses in Cu2ZnSnS4 solar cells. Applied Physics Letters, 2017, 110, .	3.3	35
10	First-principles electron transport with phonon coupling: Large scale at low cost. Physical Review B, 2017, 96, .	3.2	41
11	New approaches for first-principles modelling of inelastic transport in nanoscale semiconductor devices with thousands of atoms. , 2017, , .		0
12	Electron-phonon scattering from Green's function transport combined with molecular dynamics: Applications to mobility predictions. Physical Review B, 2017, 95, .	3.2	33
13	Probing electron-phonon excitations in molecular junctions by quantum interference. Scientific Reports, 2016, 6, 20899.	3.3	16
14	Inelastic vibrational signals in electron transport across graphene nanoconstrictions. Physical Review B, 2016, 93, .	3.2	15
15	First-principles method for electron-phonon coupling and electron mobility: Applications to two-dimensional materials. Physical Review B, 2016, 93, .	3.2	216
16	Performance study of strained IIIâ€“V materials for ultra-thin body transistor applications. , 2016, , .		3
17	Metal-InGaAs contact resistance calculations from first principles. , 2016, , .		4
18	Semiconductor band alignment from first principles: A new nonequilibrium Green's function method applied to the CZTSe/CdS interface for photovoltaics. , 2016, , .		7

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19	Comprehensive comparison and experimental validation of band-structure calculation methods in IIIâ€“V semiconductor quantum wells. Solid-State Electronics, 2016, 115, 92-102.	1.4	20
20	Nonequilibrium spin texture within a thin layer below the surface of current-carrying topological insulator<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:n A first-principles quantum transport study. Physical Review B, 2015, 92, .	3.2	41
21	Modeling approaches for band-structure calculation in III-V FET quantum wells. , 2015, , .		4
22	Mobility and bulk electron-phonon interaction in two-dimensional materials. , 2015, , .		2
23	First-principles simulations of nanoscale transistors. , 2015, , .		4
24	Temperature effects on quantum interference in molecular junctions. Physical Review B, 2014, 89, .	3.2	40
25	Simultaneous description of conductance and thermopower in single-molecule junctions from many-bodyab initiocalculations. Physical Review B, 2014, 90, .	3.2	5
26	Cross-conjugation and quantum interference: a general correlation?. Physical Chemistry Chemical Physics, 2014, 16, 653-662.	2.8	116
27	Quantitatively accurate calculations of conductance and thermopower of molecular junctions. Physica Status Solidi (B): Basic Research, 2013, 250, 2394-2402.	1.5	22
28	Carbon nanotubes as heat dissipaters in microelectronics. European Physical Journal B, 2013, 86, 1.	1.5	4
29	Energy level alignment and quantum conductance of functionalized metal-molecule junctions: Density functional theory versus GW calculations. Journal of Chemical Physics, 2013, 139, 184307.	3.0	35
30	Phonon interference effects in molecular junctions. Journal of Chemical Physics, 2013, 139, 244101.	3.0	32
31	Graphene antidot lattice waveguides. Physical Review B, 2012, 86, .	3.2	43
32	Thermoelectric properties of disordered graphene antidot devices. , 2012, , .		0
33	Surface Disordered Geâ€“Si Coreâ€“Shell Nanowires as Efficient Thermoelectric Materials. Nano Letters, 2012, 12, 4698-4704.	9.1	59
34	Observation of quantum interference in molecular charge transport. Nature Nanotechnology, 2012, 7, 305-309.	31.5	465
35	First-principles quantum transport modeling of thermoelectricity in single-molecule nanojunctions with graphene nanoribbon electrodes. Journal of Computational Electronics, 2012, 11, 78-92.	2.5	57
36	Graphical prediction of quantum interference-induced transmission nodes in functionalized organic molecules. Physical Chemistry Chemical Physics, 2011, 13, 14311.	2.8	71

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37	Multiterminal single-moleculeâ€“graphene-nanoribbon junctions with the thermoelectric figure of merit optimized via evanescent mode transport and gate voltage. Physical Review B, 2011, 84, .	3.2	69
38	Controlling the transmission line shape of molecular t-stubs and potential thermoelectric applications. Journal of Chemical Physics, 2011, 135, 154109.	3.0	60
39	Thermoelectric properties of finite graphene antidot lattices. Physical Review B, 2011, 84, .	3.2	132
40	Improving transition voltage spectroscopy of molecular junctions. Physical Review B, 2011, 83, .	3.2	29
41	Robust conductance of dumbbell molecular junctions with fullerene anchoring groups. Journal of Chemical Physics, 2011, 135, 144104.	3.0	21
42	Ab initio vibrations in nonequilibrium nanowires. Journal of Physics: Conference Series, 2010, 220, 012010.	0.4	1
43	Scattering cross section of metal catalyst atoms in silicon nanowires. Physical Review B, 2010, 81, .	3.2	9
44	Quantifying transition voltage spectroscopy of molecular junctions:Ab initiocalculations. Physical Review B, 2010, 82, .	3.2	60
45	Electrochemical control of quantum interference in anthraquinone-based molecular switches. Journal of Chemical Physics, 2010, 132, 224104.	3.0	98
46	The Relation between Structure and Quantum Interference in Single Molecule Junctions. Nano Letters, 2010, 10, 4260-4265.	9.1	296
47	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
48	Electron and phonon transport in silicon nanowires: Atomistic approach to thermoelectric properties. Physical Review B, 2009, 79, .	3.2	173
49	Electronic transport properties of fullerene functionalized carbon nanotubes:Ab initioand tight-binding calculations. Physical Review B, 2009, 80, .	3.2	30
50	Transport in silicon nanowires: role of radial dopant profile. Journal of Computational Electronics, 2008, 7, 324-327.	2.5	15
51	Heat Conductance Is Strongly Anisotropic for Pristine Silicon Nanowires. Nano Letters, 2008, 8, 3771-3775.	9.1	90
52	Modeling Transport in Ultrathin Si Nanowires: Charged versus Neutral Impurities. Nano Letters, 2008, 8, 2825-2828.	9.1	34
53	Scaling Theory Put into Practice: First-Principles Modeling of Transport in Doped Silicon Nanowires. Physical Review Letters, 2007, 99, 076803.	7.8	112
54	Influence of wetting-layer wave functions on phonon-mediated carrier capture into self-assembled quantum dots. Physical Review B, 2006, 74, .	3.2	29

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55	Electronic transport through Si nanowires: Role of bulk and surface disorder. Physical Review B, 2006, 74, .	3.2	95
56	An algebraic algorithm for generation of three-dimensional grain maps based on diffraction with a wide beam of hard X-rays. Journal of Applied Crystallography, 2004, 37, 96-102.	4.5	22