Kurt Stokbro

List of Publications by Year
in descending order

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35 papers	8,115 citations	236833 25 h-index	414303 32 g-index
35 all docs	35 docs citations	35 times ranked	6068 citing authors

#	Article	IF	Citations
1	Schottky barrier lowering due to interface states in 2D heterophase devices. Nanoscale Advances, 2021, 3, 567-574.	2.2	8
2	QuantumATK: an integrated platform of electronic and atomic-scale modelling tools. Journal of Physics Condensed Matter, 2020, 32, 015901.	0.7	771
3	First-Principles Quantum Transport Modeling of Spin-Transfer and Spin-Orbit Torques in Magnetic Multilayers. , 2020, , 499-533.		2
4	First-Principles Quantum Transport Modeling of Spin-Transfer and Spin-Orbit Torques in Magnetic Multilayers. , 2018, , 1-35.		6
5	Method for determining optimal supercell representation of interfaces. Journal of Physics Condensed Matter, 2017, 29, 185901.	0.7	59
6	ATK-ForceField: a new generation molecular dynamics software package. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 085007.	0.8	77
7	First-principles electron transport with phonon coupling: Large scale at low cost. Physical Review B, 2017, 96, .	1.1	41
8	Determination of low-strain interfaces via geometric matching. Physical Review B, 2017, 96, .	1.1	47
9	Proximity Band Structure and Spin Textures on Both Sides of Topological-Insulator/Ferromagnetic-Metal Interface and Their Charge Transport Probes. Nano Letters, 2017, 17, 5626-5633.	4.5	59
10	First-principles Green's-function method for surface calculations: A pseudopotential localized basis set approach. Physical Review B, 2017, 96, .	1.1	211
11	Complex band structure and electronic transmission eigenchannels. Journal of Chemical Physics, 2017, 147, 224104.	1.2	11
12	General atomistic approach for modeling metal-semiconductor interfaces using density functional theory and nonequilibrium Green's function. Physical Review B, 2016, 93, .	1.1	137
13	Comprehensive comparison and experimental validation of band-structure calculation methods in IIIâ€“V semiconductor quantum wells. Solid-State Electronics, 2016, 115, 92-102.	0.8	20
14	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:m A first-principles quantum transport study. Physical Review B, 2015, 92, .	1.1	41
15	Improved initial guess for minimum energy path calculations. Journal of Chemical Physics, 2014, 140, 214106.	1.2	279
16	Atomistic modeling of semiconductor interfaces. Journal of Computational Electronics, 2013, 12, 623-637.	1.3	4
17	Atomic-scale model for the contact resistance of the nickel-graphene interface. Physical Review B, 2012, 85, .	1.1	51
18	Towards realistic atomic-scale modeling of nanoscale devices. , 2011, , .		3

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19	Semiempirical model for nanoscale device simulations. Physical Review B, 2010, 82, .	1.1	158
20	First-Principles Modeling of Molecular Single-Electron Transistors. Journal of Physical Chemistry C, 2010, 114, 20461-20465.	1.5	71
21	A hybrid method for the parallel computation of Greenâ€™s functions. Journal of Computational Physics, 2009, 228, 5020-5039.	1.9	30
22	Block tridiagonal matrix inversion and fast transmission calculations. Journal of Computational Physics, 2008, 227, 3174-3190.	1.9	30
23	Krylov subspace method for evaluating the self-energy matrices in electron transport calculations. Physical Review B, 2008, 77, .	1.1	37
24	Charge Transport in Conjugated Aromatic Molecular Junctions:â€‰ Molecular Conjugation and Moleculeâ^'Electrode Coupling. Journal of Physical Chemistry C, 2007, 111, 14893-14902.	1.5	91
25	Electronic transport in crystalline magnetotunnel junctions: effects of structural disorder. Journal of Computer-Aided Materials Design, 2007, 14, 141-149.	0.7	8
26	Optical constants and self-assembly of phenylene ethynylene oligomer monolayers. Organic Electronics, 2004, 5, 315-320.	1.4	8
27	Scanning Tunneling Microscopy of Self-Assembled Phenylene Ethynylene Oligomers on Au(111) Substrates. Journal of the American Chemical Society, 2004, 126, 1229-1234.	6.6	57
28	TranSIESTA: A Spice for Molecular Electronics. Annals of the New York Academy of Sciences, 2003, 1006, 212-226.	1.8	205
29	Scanning tunneling spectroscopy of CdSe nanocrystals covalently bound to GaAs. Surface Science, 2003, 532-535, 795-800.	0.8	10
30	Do Aviramâ^'Ratner Diodes Rectify?. Journal of the American Chemical Society, 2003, 125, 3674-3675.	6.6	237
31	Conductance switching in a molecular device: The role of side groups and intermolecular interactions. Physical Review B, 2003, 68, .	1.1	191
32	Theory of Rectification in Tour Wires: The Role of Electrode Coupling. Physical Review Letters, 2002, 89, 138301.	2.9	327
33	Self-Assembled Monolayers of CdSe Nanocrystals on Doped GaAs Substrates. Nano Letters, 2002, 2, 911-914.	4.5	37
34	Simulations of quantum transport in nanoscale systems: application to atomic gold and silver wires. Nanotechnology, 2002, 13, 346-351.	1.3	39
35	Density-functional method for nonequilibrium electron transport. Physical Review B, 2002, 65, .	1.1	4,752