

Kurt Stokbro

List of Publications by Year in descending order

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Version: 2024-02-01

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	Density-functional method for nonequilibrium electron transport. <i>Physical Review B</i> , 2002, 65, .	1.1	4,752
2	QuantumATK: an integrated platform of electronic and atomic-scale modelling tools. <i>Journal of Physics Condensed Matter</i> , 2020, 32, 015901.	0.7	771
3	Theory of Rectification in Tour Wires: The Role of Electrode Coupling. <i>Physical Review Letters</i> , 2002, 89, 138301.	2.9	327
4	Improved initial guess for minimum energy path calculations. <i>Journal of Chemical Physics</i> , 2014, 140, 214106.	1.2	279
5	Do Aviram-Ratner Diodes Rectify?. <i>Journal of the American Chemical Society</i> , 2003, 125, 3674-3675.	6.6	237
6	First-principles Green's-function method for surface calculations: A pseudopotential localized basis set approach. <i>Physical Review B</i> , 2017, 96, .	1.1	211
7	TranSIESTA: A Spice for Molecular Electronics. <i>Annals of the New York Academy of Sciences</i> , 2003, 1006, 212-226.	1.8	205
8	Conductance switching in a molecular device: The role of side groups and intermolecular interactions. <i>Physical Review B</i> , 2003, 68, .	1.1	191
9	Semiempirical model for nanoscale device simulations. <i>Physical Review B</i> , 2010, 82, .	1.1	158
10	General atomistic approach for modeling metal-semiconductor interfaces using density functional theory and nonequilibrium Green's function. <i>Physical Review B</i> , 2016, 93, .	1.1	137
11	Charge Transport in Conjugated Aromatic Molecular Junctions: Molecular Conjugation and Molecular-Electrode Coupling. <i>Journal of Physical Chemistry C</i> , 2007, 111, 14893-14902.	1.5	91
12	ATK-ForceField: a new generation molecular dynamics software package. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2017, 25, 085007.	0.8	77
13	First-Principles Modeling of Molecular Single-Electron Transistors. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20461-20465.	1.5	71
14	Method for determining optimal supercell representation of interfaces. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 185901.	0.7	59
15	Proximity Band Structure and Spin Textures on Both Sides of Topological-Insulator/Ferromagnetic-Metal Interface and Their Charge Transport Probes. <i>Nano Letters</i> , 2017, 17, 5626-5633.	4.5	59
16	Scanning Tunneling Microscopy of Self-Assembled Phenylene Ethynylene Oligomers on Au(111) Substrates. <i>Journal of the American Chemical Society</i> , 2004, 126, 1229-1234.	6.6	57
17	Atomic-scale model for the contact resistance of the nickel-graphene interface. <i>Physical Review B</i> , 2012, 85, .	1.1	51
18	Determination of low-strain interfaces via geometric matching. <i>Physical Review B</i> , 2017, 96, .	1.1	47

#	ARTICLE	IF	CITATIONS
19	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:mrow></mml:math> A first-principles quantum transport study. Physical Review B, 2015, 92, .	1.1	41
20	First-principles electron transport with phonon coupling: Large scale at low cost. Physical Review B, 2017, 96, .	1.1	41
21	Simulations of quantum transport in nanoscale systems: application to atomic gold and silver wires. Nanotechnology, 2002, 13, 346-351.	1.3	39
22	Self-Assembled Monolayers of CdSe Nanocrystals on Doped GaAs Substrates. Nano Letters, 2002, 2, 911-914.	4.5	37
23	Krylov subspace method for evaluating the self-energy matrices in electron transport calculations. Physical Review B, 2008, 77, .	1.1	37
24	Block tridiagonal matrix inversion and fast transmission calculations. Journal of Computational Physics, 2008, 227, 3174-3190.	1.9	30
25	A hybrid method for the parallel computation of Greenâ€™s functions. Journal of Computational Physics, 2009, 228, 5020-5039.	1.9	30
26	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
27	Complex band structure and electronic transmission eigenchannels. Journal of Chemical Physics, 2017, 147, 224104.	1.2	11
28	Scanning tunneling spectroscopy of CdSe nanocrystals covalently bound to GaAs. Surface Science, 2003, 532-535, 795-800.	0.8	10
29	Optical constants and self-assembly of phenylene ethynylene oligomer monolayers. Organic Electronics, 2004, 5, 315-320.	1.4	8
30	Electronic transport in crystalline magnetotunnel junctions: effects of structural disorder. Journal of Computer-Aided Materials Design, 2007, 14, 141-149.	0.7	8
31	Schottky barrier lowering due to interface states in 2D heterophase devices. Nanoscale Advances, 2021, 3, 567-574.	2.2	8
32	First-Principles Quantum Transport Modeling of Spin-Transfer and Spin-Orbit Torques in Magnetic Multilayers. , 2018, , 1-35.		6
33	Atomistic modeling of semiconductor interfaces. Journal of Computational Electronics, 2013, 12, 623-637.	1.3	4
34	Towards realistic atomic-scale modeling of nanoscale devices. , 2011, , .		3
35	First-Principles Quantum Transport Modeling of Spin-Transfer and Spin-Orbit Torques in Magnetic Multilayers. , 2020, , 499-533.		2