Mark S Hybertsen

List of Publications by Year
in descending order

189	28,923	8172 76	4770 169
papers	citations	h-index	g-index

195	195	195	21647
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electron correlation in semiconductors and insulators: Band gaps and quasiparticle energies. Physical Review B, 1986, 34, 5390-5413.	1.1	3,310
2	Exciton Binding Energy and Nonhydrogenic Rydberg Series in Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>WS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:m Physical Review Letters, 2014, 113, 076802.	2.9	1,814
3	Dependence of single-molecule junction conductance on molecular conformation. Nature, 2006, 442, 904-907.	13.7	1,253
4	First-Principles Theory of Quasiparticles: Calculation of Band Gaps in Semiconductors and Insulators. Physical Review Letters, 1985, 55, 1418-1421.	2.9	1,208
5	Visualizing Individual Nitrogen Dopants in Monolayer Graphene. Science, 2011, 333, 999-1003.	6.0	774
6	Graphene Oxidation: Thickness-Dependent Etching and Strong Chemical Doping. Nano Letters, 2008, 8, 1965-1970.	4.5	773
7	Renormalization of Molecular Electronic Levels at Metal-Molecule Interfaces. Physical Review Letters, 2006, 97, 216405.	2.9	769
8	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. Physical Review B, 2013, 88, .	1.1	737
9	Single-Molecule Circuits with Well-Defined Molecular Conductance. Nano Letters, 2006, 6, 458-462.	4.5	734
10	Calculation of Coulomb-interaction parameters forLa2CuO4using a constrained-density-functional approach. Physical Review B, 1989, 39, 9028-9041.	1.1	720
11	Mechanically controlled binary conductance switching of a single-molecule junction. Nature Nanotechnology, 2009, 4, 230-234.	15.6	609
12	High-resolution scanning tunneling microscopy imaging of mesoscopic graphene sheets on an insulating surface. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9209-9212.	3.3	553
13	Observation of biexcitons in monolayer WSe2. Nature Physics, 2015, 11, 477-481.	6.5	531
14	Connecting Dopant Bond Type with Electronic Structure in N-Doped Graphene. Nano Letters, 2012, 12, 4025-4031.	4.5	471
15	Electronic states inLa2â^'xSrxCuO4+Î´probed by soft-x-ray absorption. Physical Review Letters, 1991, 66, 104-107.	2.9	463
16	Amineâ^'Gold Linked Single-Molecule Circuits:â€‰ Experiment and Theory. Nano Letters, 2007, 7, 3477-3482.	4.5	447
17	Renormalization from density-functional theory to strong-coupling models for electronic states in Cu-O materials. Physical Review B, 1990, 41, 11068-11072.	1.1	431
18	Absorption and emission of light in nanoscale silicon structures. Physical Review Letters, 1994, 72, 1514-1517.	2.9	378

#	Article	IF	Citations
19	Contact Chemistry and Single-Molecule Conductance:â€‰ A Comparison of Phosphines, Methyl Sulfides, and Amines. Journal of the American Chemical Society, 2007, 129, 15768-15769.	6.6	352
20	Ab initiostatic dielectric matrices from the density-functional approach. I. Formulation and application to semiconductors and insulators. Physical Review B, 1987, 35, 5585-5601.	1.1	338
21	Observation of Excitonic Rydberg States in Monolayer MoS₂ and WS₂ by Photoluminescence Excitation Spectroscopy. Nano Letters, 2015, 15, 2992-2997.	4.5	327
22	Electronic band structure ofCaBi2Sr2Cu2O8. Physical Review Letters, 1988, 60, 1661-1664.	2.9	319
23	Microscopic theory of singlet exciton fission. II. Application to pentacene dimers and the role of superexchange. Journal of Chemical Physics, 2013, 138, 114103.	1.2	311
24	Electronics and Chemistry:Â Varying Single-Molecule Junction Conductance Using Chemical Substituents. Nano Letters, 2007, 7, 502-506.	4.5	306
25	Probing the conductance superposition law in single-molecule circuits with parallel paths. Nature Nanotechnology, 2012, 7, 663-667.	15.6	302
26	Exciton Condensate in Semiconductor Quantum Well Structures. Physical Review Letters, 1995, 74, 1633-1636.	2.9	279
27	Tailoring the Electronic Structure in Bilayer Molybdenum Disulfide via Interlayer Twist. Nano Letters, 2014, 14, 3869-3875.	4.5	278
28	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. Accounts of Chemical Research, 2013, 46, 1321-1329.	7.6	262
29	Structure and Electronic Properties of Graphene Nanoislands on Co(0001). Nano Letters, 2009, 9, 2844-2848.	4.5	236
30	In situ formation of highly conducting covalent Auâ€“C contacts for single-molecule junctions. Nature Nanotechnology, 2011, 6, 353-357.	15.6	235
31	Formation and Evolution of Single-Molecule Junctions. Physical Review Letters, 2009, 102, 126803.	2.9	231
32	Interface structure between silicon and its oxide by first-principles molecular dynamics. Nature, 1998, 396, 58-60.	13.7	230
33	Electronic Structure of Few-Layer Epitaxial Graphene on Ru(0001). Nano Letters, 2009, 9, 2654-2660.	4.5	219
34	Theory of Si 2pcore-level shifts at the Si(001)-SiO2interface. Physical Review B, 1996, 53, 10942-10950.	1.1	211
35	Microscopic theory of singlet exciton fission. I. General formulation. Journal of Chemical Physics, 2013, 138, 114102.	1.2	210
36	Theory of optical transitions in Si/Ge(001) strained-layer superlattices. Physical Review B, 1987, 36, 9683-9693.	1.1	198

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37	Observation of Graphene Bubbles and Effective Mass Transport under Graphene Films. Nano Letters, 2009, 9, 332-337.	4.5	198
38	Quasiparticle and optical properties of rutile and anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2010, 82, .	1.1	192
39	Local Atomic and Electronic Structure of Boron Chemical Doping in Monolayer Graphene. Nano Letters, 2013, 13, 4659-4665.	4.5	192
40	Conductance and Geometry of Pyridine-Linked Single-Molecule Junctions. Journal of the American Chemical Society, 2010, 132, 6817-6821.	6.6	186
41	Van der Waals interactions at metal/organic interfaces at the single-molecule level. Nature Materials, 2012, 11, 872-876.	13.3	181
42	Si2pCore-Level Shifts at the Si(001)-SiO2Interface: A First-Principles Study. Physical Review Letters, 1995, 74, 1024-1027.	2.9	179
43	Highly Conducting Ï€-Conjugated Molecular Junctions Covalently Bonded to Gold Electrodes. Journal of the American Chemical Society, 2011, 133, 17160-17163.	6.6	169
44	Theory of quasiparticle energies in alkali metals. Physical Review Letters, 1987, 59, 819-822.	2.9	168
45	Microscopic theory of singlet exciton fission. III. Crystalline pentacene. Journal of Chemical Physics, 2014, 141, 074705.	1.2	160
46	Model dielectric matrices for quasiparticle self-energy calculations. Physical Review B, 1988, 37, 2733-2736.	1.1	155
47	Spin-orbit splitting in semiconductors and insulators from theab initiopseudopotential. Physical Review B, 1986, 34, 2920-2922.	1.1	147
48	Many-body calculation of the surface-state energies for Si(111)2Ã—1. Physical Review Letters, 1991, 66, 500-503.	2.9	138
49	Mechanics and Chemistry: Single Molecule Bond Rupture Forces Correlate with Molecular Backbone Structure. Nano Letters, 2011, 11, 1518-1523.	4.5	129
50	Theory of quasiparticle surface states in semiconductor surfaces. Physical Review B, 1988, 38, 4033-4044.	1.1	127
51	Length-Dependent Thermopower of Highly Conducting Auâ€“C Bonded Single Molecule Junctions. Nano Letters, 2013, 13, 2889-2894.	4.5	125
52	Geometric and Local Electronic Structure of Si(111)-As. Physical Review Letters, 1988, 60, 116-119.	2.9	124
53	Quantum Cascade Lasers without Intersubband Population Inversion. Physical Review Letters, 1996, 76, 411-414.	2.9	123
54	Model for low-energy electronic states probed by x-ray absorption in high-Tccuprates. Physical Review B, 1992, 45, 10032-10050.	1.1	121

#	Article	IF	Citations
55	Linker Dependent Bond Rupture Force Measurements in Single-Molecule Junctions. Journal of the American Chemical Society, 2012, 134, 4003-4006.	6.6	121
56	Electronic Structure of Tubular Aromatic Molecules Derived from the Metallic (5,5) Armchair Single Wall Carbon Nanotube. Journal of the American Chemical Society, 2004, 126, 3597-3607.	6.6	118
57	Multiphonon Relaxation Slows Singlet Fission in Crystalline Hexacene. Journal of the American Chemical Society, 2014, 136, 10654-10660.	6.6	114
58	Structurally relaxed models of the Si(001)â€“SiO2 interface. Applied Physics Letters, 1996, 68, 625-627.	1.5	110
59	Flicker Noise as a Probe of Electronic Interaction at Metalâ€“Single Molecule Interfaces. Nano Letters, 2015, 15, 4143-4149.	4.5	109
60	Absorption and luminescence studies of free-standing porous silicon films. Physical Review B, 1994, 49, 5386-5397.	1.1	106
61	Auger recombination of excitons in one-dimensional systems. Physical Review B, 2006, 73, .	1.1	105
62	Quasiparticle excitation spectrum for nearly-free-electron metals. Physical Review B, 1989, 39, 8198-8208.	1.1	103
63	First-principles analysis of electronic states in silicon nanoscale quantum wires. Physical Review B, 1993, 48, 4608-4611.	1.1	101
64	Many-body calculation of surface states: As on Ge(111). Physical Review Letters, 1987, 58, 1551-1554.	2.9	98
65	Electron correlation and the band gap in ionic crystals. Physical Review B, 1985, 32, 7005-7008.	1.1	97
66	Amine-linked single-molecule circuits: systematic trends across molecular families. Journal of Physics Condensed Matter, 2008, 20, 374115.	0.7	95
67	Quasiparticle calculation of valence band offset of AlAs-GaAs(001). Solid State Communications, 1988, 66, 585-588.	0.9	91
68	Frustrated Rotations in Single-Molecule Junctions. Journal of the American Chemical Society, 2009, 131, 10820-10821.	6.6	89
69	Binding energies and spatial structures of small carrier complexes in monolayer transition-metal dichalcogenides via diffusion Monte Carlo. Physical Review B, 2015, 92, .	1.1	88
70	Core-level photoemission measurements of valence-band offsets in highly strained heterojunctions: Si-Ge system. Physical Review B, 1989, 39, 1235-1241.	1.1	86
71	Transition Structure at theSi(100)â^'SiO2Interface. Physical Review Letters, 2003, 90, 186101.	2.9	86
72	Scanning Tunneling Microscopy Images of Alkane Derivatives on Graphite: Role of Electronic Effects. Nano Letters, 2008, 8, 3160-3165.	4.5	86

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73	Conductance of Molecular Junctions Formed with Silver Electrodes. Nano Letters, 2013, 13, 3358-3364.	4.5	86
74	Segregation of Sublattice Domains in Nitrogen-Doped Graphene. Journal of the American Chemical Society, 2014, 136, 1391-1397.	6.6	86
75	Nonlocal-density-functional approximation for exchange and correlation in semiconductors. Physical Review B, 1984, 30, 5777-5790.	1.1	83
76	Local empirical pseudopotential approach to the optical properties of Si/Ge superlattices. Physical Review B, 1989, 39, 7974-7977.	1.1	83
77	Analysis of gain in determining T/sub 0/ in 1.3 Î¼m semiconductor lasers. IEEE Journal of Selected Topics in Quantum Electronics, 1995, 1, 250-263.	1.9	77
78	Single-Molecule Junction Conductance through Diaminoacenes. Journal of the American Chemical Society, 2007, 129, 6714-6715.	6.6	76
79	Forming Aromatic Hemispheres on Transitionâ€Metal Surfaces. Angewandte Chemie - International Edition, 2007, 46, 7891-7895.	7.2	76
80	Photocatalytic Water Oxidation at the GaN (101Ì…0)â^'Water Interface. Journal of Physical Chemistry C, 2010, 114, 13695-13704.	1.5	74
81	First-Principles Approach to Calculating Energy Level Alignment at Aqueous Semiconductor Interfaces. Physical Review Letters, 2014, 113, 176802.	2.9	72
82	Band offset transitivity at the InGaAs/InAlAs/InP(001) heterointerfaces. Applied Physics Letters, 1991, 58, 1759-1761.	1.5	70
83	Evaluation of quasiparticle energies for semiconductors without inversion symmetry. Physical Review B, 1989, 40, 3162-3168.	1.1	69
84	Formation of Catalytic Metal-Molecule Contacts. Science, 2005, 309, 591-594.	6.0	69
85	Bright and dark singlet excitons via linear and two-photon spectroscopy in monolayer transition-metal dichalcogenides. Physical Review B, 2015, 92, .	1.1	68
86	Structureâ€“Property Relationships in Atomic-Scale Junctions: Histograms and Beyond. Accounts of Chemical Research, 2016, 49, 452-460.	7.6	65
87	Determination of the structure and geometry of N-heterocyclic carbenes on Au(111) using high-resolution spectroscopy. Chemical Science, 2019, 10, 930-935.	3.7	64
88	Ab initiostatic dielectric matrices from the density-functional approach. II. Calculation of the screening response in diamond, Si, Ge, and LiCl. Physical Review B, 1987, 35, 5602-5610.	1.1	62
89	Structural and chemical trends in doped silicon nanocrystals: First-principles calculations. Physical Review B, 2005, 71, .	1.1	62
90	Role of interface strain in a lattice-matched heterostructure. Physical Review Letters, 1990, 64, 555-558.	2.9	55

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91	Negative Differential Resistance in Transport through Organic Molecules on Silicon. Physical Review Letters, 2007, 98, 066807.	2.9	54
92	Location of atoms in the first monolayer of GaAs on Si. Physical Review Letters, 1987, 59, 2180-2183.	2.9	53
93	Monolayer growth and structure of ga on si(111). Physical Review B, 1988, 38, 7885-7888.	1.1	53
94	Electronic correlation in nanoscale junctions: Comparison of the GW approximation to a numerically exact solution of the single-impurity Anderson model. Physical Review B, 2008, 77, .	1.1	53
95	Atomistic Interrogation of Bâ€“N Co-dopant Structures and Their Electronic Effects in Graphene. ACS Nano, 2016, 10, 6574-6584.	7.3	53
96	40-Gb/s tandem electroabsorption modulator. IEEE Photonics Technology Letters, 2002, 14, 27-29.	1.3	52
97	Visualization of lithium-ion transport and phase evolution within and between manganese oxide nanorods. Nature Communications, 2017, 8, 15400.	5.8	52
98	Water Adsorption on the GaN (101Ì…0) Nonpolar Surface. Journal of Physical Chemistry C, 2009, 113, 3365-3368.	1.5	51
99	GW approach to Anderson model out of equilibrium: Coulomb blockade and false hysteresis in thelâ^Vcharacteristics. Physical Review B, 2009, 79, .	1.1	51
100	Comparison of structurally relaxed models of the Si(001)-SiO2 interface based on different crystalline oxide forms. Applied Surface Science, 1996, 104-105, 317-322.	3.1	50
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109	Enhanced static approximation to the electron self-energy operator for efficient calculation of quasiparticle energies. Physical Review B, 2010, 82, .	1.1	42
110	Role of p-doping profile and regrowth on the static characteristics of 1.3-Î¼m MQW InGaAsP-InP lasers: experiment and modeling. IEEE Journal of Quantum Electronics, 1999, 35, 1515-1520.	1.0	40
111	Computational investigation of structural and electronic properties of aqueous interfaces of GaN, ZnO, and a GaN/ZnO alloy. Physical Chemistry Chemical Physics, 2014, 16, 12057-12066.	1.3	39
112	Semiconductorâ€Based Photoelectrochemical Water Splitting at the Limit of Very Wide Depletion Region. Advanced Functional Materials, 2016, 26, 219-225.	7.8	39
113	Impedanceâ€corrected carrier lifetime measurements in semiconductor lasers. Applied Physics Letters, 1995, 67, 1506-1508.	1.5	38
114	SpherosiloxaneH8Si8O12clusters on Si(001): First-principles calculation of Si2pcore-level shifts. Physical Review B, 1996, 54, R2339-R2342.	1.1	38
115	Reliable Formation of Single Molecule Junctions with Air-Stable Diphenylphosphine Linkers. Journal of Physical Chemistry Letters, 2010, 1, 2114-2119.	2.1	38
116	Frustrated Ostwald Ripening in Self-Assembled Monolayers of Cruciform Ï€-Systems. Langmuir, 2006, 22, 10003-10008.	1.6	37
117	Calculation of the many body interaction parameters in the highTc compound La2CuO4. Physica C: Superconductivity and Its Applications, 1988, 153-155, 1217-1218.	0.6	36
118	Performance of carbon nanotube-dispersed thin-film transistors. Applied Physics Letters, 2006, 89, 143501.	1.5	36
119	A Physical Model for Understanding the Activation of MoS₂ Basalâ€Plane Sulfur Atoms for the Hydrogen Evolution Reaction. Angewandte Chemie - International Edition, 2020, 59, 14835-14841.	7.2	36
120	Non-local density functional theory for the electronic and structural properties of semiconductors. Solid State Communications, 1984, 51, 451-454.	0.9	34
121	The Electrical Properties of Biphenylenes. Organic Letters, 2010, 12, 4114-4117.	2.4	34
122	Fully stabilized electroabsorption-modulated tunable DBR laser transmitter for long-haul optical communications. IEEE Journal of Selected Topics in Quantum Electronics, 2001, 7, 168-177.	1.9	33
123	Photoinduced Water Oxidation at the Aqueous GaN (101Ì…0) Interface: Deprotonation Kinetics of the First Proton-Coupled Electron-Transfer Step. ACS Catalysis, 2015, 5, 2317-2323.	5.5	33
124	Simulation of semiconductor quantum well lasers. IEEE Transactions on Electron Devices, 2000, 47, 1917-1925.	1.6	31
125	Microscopic relaxation channels in materials for superconducting qubits. Communications Materials, 2021, 2, .	2.9	31
126	Piezoreflectance study of short-period strained Si-Ge superlattices grown on (001) Ge. Physical Review B, 1991, 44, 5955-5957.	1.1	29

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127	Controlled Growth of Ceria Nanoarrays on Anatase Titania Powder: A Bottom-up Physical Picture. Nano Letters, 2017, 17, 348-354.	4.5	29
128	Electron-hole system revisited: A variational quantum Monte Carlo study. Physical Review B, 1996, 54, 13575-13580.	1.1	28
129	Density-Functional Study of Adsorption of Isocyanides on a Gold (111) Surface. Journal of Physical Chemistry C, 2008, 112, 3314-3320.	1.5	27
130	Analysis of T0 in 1.3 Î¼m multiâ€quantumâ€well and bulk active lasers. Applied Physics Letters, 1995, 66, 2613-2615.	1.5	26
131	Energetics of Lithium Insertion into Magnetite, Defective Magnetite, and Maghemite. Chemistry of Materials, 2018, 30, 7922-7937.	3.2	26
132	Graphite, Tubular PAHs, and the Diffuse Interstellar Bands. Astrophysical Journal, 2006, 638, L105-L108.	1.6	25
133	Temperature dependence of the fundamental direct transitions of bulk Ge and two Ge/SiGe multiple-quantum-well structures. Physical Review B, 1995, 52, 8951-8958.	1.1	21
134	Growth and structural analysis of an ordered boron monolayer in Si(100). Physical Review B, 1992, 46, 12861-12864.	1.1	20
135	Interface strain at the lattice-matched In0.53Ga0.47As/InP(001) heterointerface. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1990, 8, 773.	1.6	19
136	First-principles study of Siâ€‰2p core-level shifts at water and hydrogen covered Si(001)2Ã—1 surfaces. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1996, 14, 2809.	1.6	18
137	Si 2p core-level shifts in small molecules: a first principles study. Physica Scripta, 1996, T66, 118-120.	1.2	17
138	Quantitative Bond Energetics in Atomic-Scale Junctions. ACS Nano, 2014, 8, 7522-7530.	7.3	17
139	Charge localization and ordering in A2Mn8O16 hollandite group oxides: Impact of density functional theory approaches. Physical Review Materials, 2017, 1, .	0.9	17
140	An Intrinsic Model for Radiative Recombination in Porous Silicon. Materials Research Society Symposia Proceedings, 1991, 256, 179.	0.1	16
141	Chemisorption pathways and Siâ€Š2p core-level shifts for the interaction of spherosiloxane clusters with Si(100): Implications for photoemission in Si/SiO2 systems. Applied Physics Letters, 2000, 76, 3873-3875.	1.5	16
142	Theoretical study of trends in conductance for molecular junctions formed with armchair carbon nanotube electrodes. Physical Review B, 2007, 76, .	1.1	16
143	Effect of p-doping on the temperature dependence of differential gain in FP and DFB 1.3-Î¼m InGaAsP-InP multiple-quantum-well lasers. IEEE Photonics Technology Letters, 2000, 12, 969-971.	1.3	14
144	Atomic Scale Account of the Surface Effect on Ionic Transport in Silver Hollandite. Chemistry of Materials, 2018, 30, 6124-6133.	3.2	14

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145	Ultrathin Amorphous Titania on Nanowires: Optimization of Conformal Growth and Elucidation of Atomic-Scale Motifs. Nano Letters, 2019, 19, 3457-3463.	4.5	14
146	The electronic structure of La 2 CuO 4 : Renormalization from density functional theory to strong coupling models. Physica C: Superconductivity and Its Applications, 1989, 162-164, 583-586.	0.6	13
147	A theoretical investigation of the characteristic temperature T/sub 0/ for semiconductor lasers. IEEE Journal of Selected Topics in Quantum Electronics, 2003, 9, 807-815.	1.9	13
148	Resolving the Evolution of Atomic Layer-Deposited Thin-Film Growth by Continuous In Situ X-Ray Absorption Spectroscopy. Chemistry of Materials, 2021, 33, 1740-1751.	3.2	13
149	Formation and Evolution of Metallocene Single-Molecule Circuits with Direct Gold-Ï€ Links. Journal of the American Chemical Society, 2022, 144, 6504-6515.	6.6	13
150	Multiwavelength DFB laser array with integrated spot size converters. IEEE Journal of Quantum Electronics, 2000, 36, 641-648.	1.0	12
151	First-principles studies of the electronic structure of cyclopentene on Si(001): density functional theory and GW calculations. Physica Status Solidi (B): Basic Research, 2006, 243, 2048-2053.	0.7	12
152	Scanning Tunneling Microscope Studies of Ultrathin Graphitic (Graphene) Films on an Insulating Substrate under Ambient Conditions. Journal of Physical Chemistry C, 2008, 112, 6681-6688.	1.5	12
153	Modeling single molecule junction mechanics as a probe of interface bonding. Journal of Chemical Physics, 2017, 146, .	1.2	11
154	Theory of quasiparticle energies: Band gaps and excitation spectra in solids. International Journal of Quantum Chemistry, 1987, 32, 31-44.	1.0	10
155	Quantum beats in photon echo from four-waving mixing. Physical Review Letters, 1994, 73, 209-209.	2.9	9
156	Microscopic simulation of the temperature dependence of static and dynamic 1.3-Î¼m multi-quantum-well laser performance. IEEE Journal of Quantum Electronics, 2003, 39, 120-129.	1.0	9
157	Solvent Effects on the Self-Assembly of 1-Bromoeicosane on Graphite. Part II. Theory. Journal of Physical Chemistry C, 2009, 113, 3641-3649.	1.5	9
158	Design of Medium Band Gap Agâ€“Biâ€“Nbâ€“O and Agâ€“Biâ€“Taâ€“O Semiconductors for Driving Direct Water Splitting with Visible Light. Inorganic Chemistry, 2013, 52, 9192-9205.	1.9	9
159	A Physical Model for Understanding the Activation of MoS₂ Basalâ€Plane Sulfur Atoms for the Hydrogen Evolution Reaction. Angewandte Chemie, 2020, 132, 14945-14951.	1.6	9
160	The Atomic and Electronic Structure of Ordered Buried B(2x1) Layers in Si(100). Materials Science Forum, 1992, 83-87, 1391-1396.	0.3	8
161	Dopant local bonding and electrical activity near Si(001)-oxide interfaces. Journal of Applied Physics, 2005, 98, 076105.	1.1	8
162	Charge Disproportionation in Tetragonal La₂MoO₅, a Small Band Gap Semiconductor Influenced by Direct Moâ€“Mo Bonding. Journal of the American Chemical Society, 2015, 137, 1245-1257.	6.6	8

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163	Description of quasiparticle and satellite properties via cumulant expansions of the retarded one-particle Green's function. Physical Review B, 2016, 94, .	1.1	8
164	Self-Energy Approach to Quasiparticle Energies Using a Density Functional Treatment of Dielectric Screening. Advances in Quantum Chemistry, 1990, , 155-174.	0.4	7
165	Microscopic theory of heterojunction band offsets. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1992, 14, 254-261.	1.7	7
166	Four-wave mixing and terahertz emission from three-level systems in quantum wells: Effects of inhomogeneous broadening. Physical Review B, 1994, 50, 11915-11923.	1.1	7
167	Excitation and characterization of image potential state electrons on quasi-free-standing graphene. Physical Review B, 2018, 97, .	1.1	7
168	Probing Structural Reconstruction of Metal Nanoparticles under Annealing and Water Vapor Conditions: A Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 29783-29793.	1.5	7
169	Observation of intercalation-driven zone folding in quasi-free-standing graphene energy bands. Physical Review B, 2019, 99, .	1.1	6
170	Hydrogen bonded trimesic acid networks on Cu(111) reveal how basic chemical properties are imprinted in HR-AFM images. Nanoscale, 2021, 13, 18473-18482.	2.8	6
171	Data-driven approach to parameterize <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>SCAN</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:m for an accurate description of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml: transition metal oxide thermochemistry. Physical Review Materials, 2022, 6, .	0.9	6
172	Core-Level Shifts in Si(001)-SiO2 Systems: The Value of First-Principle Investigations. , 1998, , 89-102.		5
173	Silicon crystal distortions at the Si(100)â€“SiO2 interface from analysis of ion-scattering. Microelectronic Engineering, 2004, 72, 197-200.	1.1	5
174	Piezoreflectance of strained Si/Ge superlattices grown on Ge(001). Surface Science, 1992, 267, 99-102.	0.8	4
175	Effects of the interfacial polarization on tunneling in surface coupled quantum dots. Physical Review B, 2012, 86, .	1.1	4
176	Excitons in atomically thin transition-metal dichalcogenides. , 2014, , .		4
177	Theory of Optical Transitions in SinGen(001) Strained Layer Superlattices. Materials Research Society Symposia Proceedings, 1987, 102, 413.	0.1	3
178	Theory of the Quasiparticle Effective Masses in Semiconductors based on an Electron Self Energy Approach. Materials Research Society Symposia Proceedings, 1990, 193, 113.	0.1	3
179	Ion scattering simulations of theSi(100)â^'SiO2interface. Physical Review B, 2006, 74, .	1.1	2
180	Renormalization from Density Functional Theory to Strong Coupling Models for the Electronic Structure of La2CuO4. Materials Research Society Symposia Proceedings, 1989, 169, 19.	0.1	1

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