Mark S Hybertsen

List of Publications by Year
in descending order

		8181	4774
189	28,923	76	169
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	Formation and Evolution of Metallocene Single-Molecule Circuits with Direct Gold-Ïϵ Links. Journal of the American Chemical Society, 2022, 144, 6504-6515.	13.7	13
2	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:m transition metal oxide thermochemistry. Physical Review Materials, 2022, 6, .	2.4	6
3	Hydrogen bonded trimesic acid networks on Cu(111) reveal how basic chemical properties are imprinted in HR-AFM images. Nanoscale, 2021, 13, 18473-18482.	5.6	6
4	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.	6.7	13
5	Microscopic relaxation channels in materials for superconducting qubits. Communications Materials, 2021, 2, .	6.9	31
6	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.	13.8	36
7	A Physical Model for Understanding the Activation of MoS₂ Basalâ€Plane Sulfur Atoms for the Hydrogen Evolution Reaction. Angewandte Chemie, 2020, 132, 14945-14951.	2.0	9
8	Determination of the structure and geometry of N-heterocyclic carbenes on Au(111) using high-resolution spectroscopy. Chemical Science, 2019, 10, 930-935.	7.4	64
9	Observation of intercalation-driven zone folding in quasi-free-standing graphene energy bands. Physical Review B, 2019, 99, .	3.2	6
10	Ultrathin Amorphous Titania on Nanowires: Optimization of Conformal Growth and Elucidation of Atomic-Scale Motifs. Nano Letters, 2019, 19, 3457-3463.	9.1	14
11	Probing Structural Reconstruction of Metal Nanoparticles under Annealing and Water Vapor Conditions: A Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 29783-29793.	3.1	7
12	Excitation and characterization of image potential state electrons on quasi-free-standing graphene. Physical Review B, 2018, 97, .	3.2	7
13	In-situ Probe of Lithium-ion Transport and Phase Evolution Within and Between Silver Hollandite Nanorods. Microscopy and Microanalysis, 2018, 24, 1516-1517.	0.4	0
14	Energetics of Lithium Insertion into Magnetite, Defective Magnetite, and Maghemite. Chemistry of Materials, 2018, 30, 7922-7937.	6.7	26
15	Atomic Scale Account of the Surface Effect on Ionic Transport in Silver Hollandite. Chemistry of Materials, 2018, 30, 6124-6133.	6.7	14
16	Modeling single molecule junction mechanics as a probe of interface bonding. Journal of Chemical Physics, 2017, 146, .	3.0	11
17	Visualization of lithium-ion transport and phase evolution within and between manganese oxide nanorods. Nature Communications, 2017, 8, 15400.	12.8	52
18	Controlled Growth of Ceria Nanoarrays on Anatase Titania Powder: A Bottom-up Physical Picture. Nano Letters, 2017, 17, 348-354.	9.1	29

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19	Charge localization and ordering in A2Mn8O16 hollandite group oxides: Impact of density functional theory approaches. Physical Review Materials, 2017, 1, .	2.4	17
20	Description of quasiparticle and satellite properties via cumulant expansions of the retarded one-particle Green's function. Physical Review B, 2016, 94, .	3.2	8
21	Semiconductorâ€Based Photoelectrochemical Water Splitting at the Limit of Very Wide Depletion Region. Advanced Functional Materials, 2016, 26, 219-225.	14.9	39
22	Atomistic Interrogation of Bâ€“N Co-dopant Structures and Their Electronic Effects in Graphene. ACS Nano, 2016, 10, 6574-6584.	14.6	53
23	Structureâ€“Property Relationships in Atomic-Scale Junctions: Histograms and Beyond. Accounts of Chemical Research, 2016, 49, 452-460.	15.6	65
24	Bright and dark singlet excitons via linear and two-photon spectroscopy in monolayer transition-metal dichalcogenides. Physical Review B, 2015, 92, .	3.2	68
25	Binding energies and spatial structures of small carrier complexes in monolayer transition-metal dichalcogenides via diffusion Monte Carlo. Physical Review B, 2015, 92, .	3.2	88
26	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.	11.2	33
27	Flicker Noise as a Probe of Electronic Interaction at Metalâ€“Single Molecule Interfaces. Nano Letters, 2015, 15, 4143-4149.	9.1	109
28	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.	13.7	8
29	Observation of biexcitons in monolayer WSe2. Nature Physics, 2015, 11, 477-481.	16.7	531
30	Observation of Excitonic Rydberg States in Monolayer MoS₂ and WS₂ by Photoluminescence Excitation Spectroscopy. Nano Letters, 2015, 15, 2992-2997.	9.1	327
31	Excitons in atomically thin transition-metal dichalcogenides. , 2014, , .		4
32	First-Principles Approach to Calculating Energy Level Alignment at Aqueous Semiconductor Interfaces. Physical Review Letters, 2014, 113, 176802.	7.8	72
33	Microscopic theory of singlet exciton fission. III. Crystalline pentacene. Journal of Chemical Physics, 2014, 141, 074705.	3.0	160
34	Segregation of Sublattice Domains in Nitrogen-Doped Graphene. Journal of the American Chemical Society, 2014, 136, 1391-1397.	13.7	86
35	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.	2.8	39
36	Multiphonon Relaxation Slows Singlet Fission in Crystalline Hexacene. Journal of the American Chemical Society, 2014, 136, 10654-10660.	13.7	114

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37	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:mrow> Physical Review Letters, 2014, 113, 076802.	7.8	1,814
38	Tailoring the Electronic Structure in Bilayer Molybdenum Disulfide via Interlayer Twist. Nano Letters, 2014, 14, 3869-3875.	9.1	278
39	Quantitative Bond Energetics in Atomic-Scale Junctions. ACS Nano, 2014, 8, 7522-7530.	14.6	17
40	Edge Structures for Nanoscale Graphene Islands on Co(0001) Surfaces. ACS Nano, 2014, 8, 5765-5773.	14.6	49
41	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.	4.0	9
42	Length-Dependent Thermopower of Highly Conducting Auâ€“C Bonded Single Molecule Junctions. Nano Letters, 2013, 13, 2889-2894.	9.1	125
43	Microscopic theory to quantify the competing kinetic processes in photoexcited surface-coupled quantum dots. Physical Review B, 2013, 87, .	3.2	0
44	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. Physical Review B, 2013, 88, .	3.2	737
45	Local Atomic and Electronic Structure of Boron Chemical Doping in Monolayer Graphene. Nano Letters, 2013, 13, 4659-4665.	9.1	192
46	Microscopic theory of singlet exciton fission. II. Application to pentacene dimers and the role of superexchange. Journal of Chemical Physics, 2013, 138, 114103.	3.0	311
47	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. Accounts of Chemical Research, 2013, 46, 1321-1329.	15.6	262
48	Microscopic theory of singlet exciton fission. I. General formulation. Journal of Chemical Physics, 2013, 138, 114102.	3.0	210
49	Simultaneous Measurement of Force and Conductance Across Single Molecule Junctions. Conference Proceedings of the Society for Experimental Mechanics, 2013, , 75-84.	0.5	0
50	Conductance of Molecular Junctions Formed with Silver Electrodes. Nano Letters, 2013, 13, 3358-3364.	9.1	86
51	Linker Dependent Bond Rupture Force Measurements in Single-Molecule Junctions. Journal of the American Chemical Society, 2012, 134, 4003-4006.	13.7	121
52	Van der Waals interactions at metal/organic interfaces at the single-molecule level. Nature Materials, 2012, 11, 872-876.	27.5	181
53	Probing the conductance superposition law in single-molecule circuits with parallel paths. Nature Nanotechnology, 2012, 7, 663-667.	31.5	302
54	Effects of the interfacial polarization on tunneling in surface coupled quantum dots. Physical Review B, 2012, 86, .	3.2	4

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55	Connecting Dopant Bond Type with Electronic Structure in N-Doped Graphene. Nano Letters, 2012, 12, 4025-4031.	9.1	471
56	Mechanics and Chemistry: Single Molecule Bond Rupture Forces Correlate with Molecular Backbone Structure. Nano Letters, 2011, 11, 1518-1523.	9.1	129
57	Highly Conducting Ï€-Conjugated Molecular Junctions Covalently Bonded to Gold Electrodes. Journal of the American Chemical Society, 2011, 133, 17160-17163.	13.7	169
58	Visualizing Individual Nitrogen Dopants in Monolayer Graphene. Science, 2011, 333, 999-1003.	12.6	774
59	In situ formation of highly conducting covalent Auâ€“C contacts for single-molecule junctions. Nature Nanotechnology, 2011, 6, 353-357.	31.5	235
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73	Observation of Graphene Bubbles and Effective Mass Transport under Graphene Films. Nano Letters, 2009, 9, 332-337.	9.1	198
74	Electronic Structure of Few-Layer Epitaxial Graphene on Ru(0001). Nano Letters, 2009, 9, 2654-2660.	9.1	219
75	GW approach to Anderson model out of equilibrium: Coulomb blockade and false hysteresis in theIâ^'Vcharacteristics. Physical Review B, 2009, 79, .	3.2	51
76	Structure and Electronic Properties of Graphene Nanoislands on Co(0001). Nano Letters, 2009, 9, 2844-2848.	9.1	236
77	Graphene Oxidation: Thickness-Dependent Etching and Strong Chemical Doping. Nano Letters, 2008, 8, 1965-1970.	9.1	773
78	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, .	3.2	53
79	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.	3.1	12
80	Scanning Tunneling Microscopy Images of Alkane Derivatives on Graphite: Role of Electronic Effects. Nano Letters, 2008, 8, 3160-3165.	9.1	86
81	Density-Functional Study of Adsorption of Isocyanides on a Gold (111) Surface. Journal of Physical Chemistry C, 2008, 112, 3314-3320.	3.1	27
82	Amine-linked single-molecule circuits: systematic trends across molecular families. Journal of Physics Condensed Matter, 2008, 20, 374115.	1.8	95
83	Negative Differential Resistance in Transport through Organic Molecules on Silicon. Physical Review Letters, 2007, 98, 066807.	7.8	54
84	Theoretical study of trends in conductance for molecular junctions formed with armchair carbon nanotube electrodes. Physical Review B, 2007, 76, .	3.2	16
85	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.	13.7	352
86	Single-Molecule Junction Conductance through Diaminoacenes. Journal of the American Chemical Society, 2007, 129, 6714-6715.	13.7	76
87	Amineâ^'Gold Linked Single-Molecule Circuits:â€‰ Experiment and Theory. Nano Letters, 2007, 7, 3477-3482.	9.1	447
88	Electronics and Chemistry:Â Varying Single-Molecule Junction Conductance Using Chemical Substituents. Nano Letters, 2007, 7, 502-506.	9.1	306
89	Auger Recombination of Excitons in Semiconducting Carbon Nanotubes. Springer Series in Chemical Physics, 2007, , 683-685.	0.2	0
90	Forming Aromatic Hemispheres on Transitionâ€Metal Surfaces. Angewandte Chemie - International Edition, 2007, 46, 7891-7895.	13.8	76

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91	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.	7.1	553
92	Renormalization of Molecular Electronic Levels at Metal-Molecule Interfaces. Physical Review Letters, 2006, 97, 216405.	7.8	769
93	Single-Molecule Circuits with Well-Defined Molecular Conductance. Nano Letters, 2006, 6, 458-462.	9.1	734
94	Frustrated Ostwald Ripening in Self-Assembled Monolayers of Cruciform Ï€-Systems. Langmuir, 2006, 22, 10003-10008.	3.5	37
95	Graphite, Tubular PAHs, and the Diffuse Interstellar Bands. Astrophysical Journal, 2006, 638, L105-L108.	4.5	25
96	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.	1.5	12
97	Dependence of single-molecule junction conductance on molecular conformation. Nature, 2006, 442, 904-907.	27.8	1,253
98	Auger recombination of excitons in one-dimensional systems. Physical Review B, 2006, 73, .	3.2	105
99	Performance of carbon nanotube-dispersed thin-film transistors. Applied Physics Letters, 2006, 89, 143501.	3.3	36
100	Ion scattering simulations of theSi(100)â^'SiO2interface. Physical Review B, 2006, 74, .	3.2	2
101	Structural and chemical trends in doped silicon nanocrystals: First-principles calculations. Physical Review B, 2005, 71, .	3.2	62
102	Dopant local bonding and electrical activity near Si(001)-oxide interfaces. Journal of Applied Physics, 2005, 98, 076105.	2.5	8
103	Formation of Catalytic Metal-Molecule Contacts. Science, 2005, 309, 591-594.	12.6	69
104	Silicon crystal distortions at the Si(100)â€“SiO2 interface from analysis of ion-scattering. Microelectronic Engineering, 2004, 72, 197-200.	2.4	5
105	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.	13.7	118
106	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.	2.9	13
107	Transition Structure at theSi(100)â^'SiO2Interface. Physical Review Letters, 2003, 90, 186101.	7.8	86
108	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.	1.9	9

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109	40-Gb/s tandem electroabsorption modulator. IEEE Photonics Technology Letters, 2002, 14, 27-29.	2.5	52
110	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.	2.9	33
111	Simulation of semiconductor quantum well lasers. IEEE Transactions on Electron Devices, 2000, 47, 1917-1925.	3.0	31
112	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.	3.3	16
113	Multiwavelength DFB laser array with integrated spot size converters. IEEE Journal of Quantum Electronics, 2000, 36, 641-648.	1.9	12
114	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.	2.5	14
115	Synchrotron x-ray microdiffraction diagnostics of multilayer optoelectronic devices. Applied Physics Letters, 1999, 75, 100-102.	3.3	45
116	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.	1.9	40
117	Simulation and characterization of the selective area growth process. Applied Physics Letters, 1999, 74, 2617-2619.	3.3	48
118	Interface structure between silicon and its oxide by first-principles molecular dynamics. Nature, 1998, 396, 58-60.	27.8	230
119	Core-Level Shifts in Si(001)-SiO2 Systems: The Value of First-Principle Investigations. , 1998, , 89-102.		5
120	Electron-hole system revisited: A variational quantum Monte Carlo study. Physical Review B, 1996, 54, 13575-13580.	3.2	28
121	Quantum Cascade Lasers without Intersubband Population Inversion. Physical Review Letters, 1996, 76, 411-414.	7.8	123
122	Theory of Si 2pcore-level shifts at the Si(001)-SiO2interface. Physical Review B, 1996, 53, 10942-10950.	3.2	211
123	Structurally relaxed models of the Si(001)â€“SiO2 interface. Applied Physics Letters, 1996, 68, 625-627.	3.3	110
124	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.	6.1	50
125	SpherosiloxaneH8Si8O12clusters on Si(001): First-principles calculation of Si2pcore-level shifts. Physical Review B, 1996, 54, R2339-R2342.	3.2	38
126	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

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127	Si 2p core-level shifts in small molecules: a first principles study. Physica Scripta, 1996, T66, 118-120.	2.5	17
128	Microscopic Theory of the Properties of Semiconductor Heterojunctions. Kluwer International Series in Engineering and Computer Science, 1996, , 189-200.	0.2	0
129	Exciton Condensate in Semiconductor Quantum Well Structures. Physical Review Letters, 1995, 74, 1633-1636.	7.8	279
130	Analysis of T0 in 1.3 Î¼m multiâ€quantumâ€well and bulk active lasers. Applied Physics Letters, 1995, 66, 2613-2615.	3.3	26
131	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.	3.2	21
132	Si2pCore-Level Shifts at the Si(001)-SiO2Interface: A First-Principles Study. Physical Review Letters, 1995, 74, 1024-1027.	7.8	179
133	Impedanceâ€corrected carrier lifetime measurements in semiconductor lasers. Applied Physics Letters, 1995, 67, 1506-1508.	3.3	38
134	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.	2.9	77
135	Implication of Silicon Nanocrystallites from Combined Absorption and Luminescence Studies of Free-Standing Porous Silicon Films. Japanese Journal of Applied Physics, 1995, 34, 257.	1.5	0
136	Quantum beats in photon echo from four-waving mixing. Physical Review Letters, 1994, 73, 209-209.	7.8	9
137	Four-wave mixing and terahertz emission from three-level systems in quantum wells: Effects of inhomogeneous broadening. Physical Review B, 1994, 50, 11915-11923.	3.2	7
138	Absorption and luminescence studies of free-standing porous silicon films. Physical Review B, 1994, 49, 5386-5397.	3.2	106
139	Absorption and emission of light in nanoscale silicon structures. Physical Review Letters, 1994, 72, 1514-1517.	7.8	378
140	First-principles analysis of electronic states in silicon nanoscale quantum wires. Physical Review B, 1993, 48, 4608-4611.	3.2	101
141	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
142	Model for low-energy electronic states probed by x-ray absorption in high-Tccuprates. Physical Review B, 1992, 45, 10032-10050.	3.2	121
143	Growth and structural analysis of an ordered boron monolayer in Si(100). Physical Review B, 1992, 46, 12861-12864.	3.2	20
144	Piezoreflectance of strained Si/Ge superlattices grown on Ge(001). Surface Science, 1992, 267, 99-102.	1.9	4

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145	Microscopic theory of heterojunction band offsets. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1992, 14, 254-261.	3.5	7
146	Models for the Electronic Structure of Cuprates. Physics and Chemistry of Materials With Low-dimensional Structures, 1992, , 229-245.	1.0	0
147	Band offset transitivity at the InGaAs/InAlAs/InP(001) heterointerfaces. Applied Physics Letters, 1991, 58, 1759-1761.	3.3	70
148	An Intrinsic Model for Radiative Recombination in Porous Silicon. Materials Research Society Symposia Proceedings, 1991, 256, 179.	0.1	16
149	Electronic states inLa2â^'xSrxCuO4+Î´probed by soft-x-ray absorption. Physical Review Letters, 1991, 66, 104-107.	7.8	463
150	Many-body calculation of the surface-state energies for Si(111)2Ã—1. Physical Review Letters, 1991, 66, 500-503.	7.8	138
151	Piezoreflectance study of short-period strained Si-Ge superlattices grown on (001) Ge. Physical Review B, 1991, 44, 5955-5957.	3.2	29
152	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
153	Self-Energy Approach to Quasiparticle Energies Using a Density Functional Treatment of Dielectric Screening. Advances in Quantum Chemistry, 1990, , 155-174.	0.8	7
154	Role of interface strain in a lattice-matched heterostructure. Physical Review Letters, 1990, 64, 555-558.	7.8	55
155	Renormalization from density-functional theory to strong-coupling models for electronic states in Cu-O materials. Physical Review B, 1990, 41, 11068-11072.	3.2	431
156	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
157	Quasiparticle band offset at the (001) interface and band gaps in ultrathin superlattices of GaAs-AlAs heterojunctions. Physical Review B, 1990, 41, 10058-10067.	3.2	42
158	Core-level photoemission measurements of valence-band offsets in highly strained heterojunctions: Si-Ge system. Physical Review B, 1989, 39, 1235-1241.	3.2	86
159	Local empirical pseudopotential approach to the optical properties of Si/Ge superlattices. Physical Review B, 1989, 39, 7974-7977.	3.2	83
160	Quasiparticle excitation spectrum for nearly-free-electron metals. Physical Review B, 1989, 39, 8198-8208.	3.2	103
161	Calculation of Coulomb-interaction parameters forLa2CuO4using a constrained-density-functional approach. Physical Review B, 1989, 39, 9028-9041.	3.2	720
162	Evaluation of quasiparticle energies for semiconductors without inversion symmetry. Physical Review B, 1989, 40, 3162-3168.	3.2	69

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163	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.	1.2	13
164	Quasiparticle band gaps for ultrathin GaAs/AlAs(001) superlattices. Physical Review Letters, 1989, 63, 1495-1498.	7.8	44
165	Interface Strain and the Valence Band Offset at the Lattice Matched In0.53Ga0.47As/InP (001) Interface. Materials Research Society Symposia Proceedings, 1989, 159, 109.	0.1	0
166	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
167	Quasiparticle calculation of valence band offset of AlAs-GaAs(001). Solid State Communications, 1988, 66, 585-588.	1.9	91
168	Calculation of the many body interaction parameters in the highTc compound La2CuO4. Physica C: Superconductivity and Its Applications, 1988, 153-155, 1217-1218.	1.2	36
169	Theory of quasiparticle surface states in semiconductor surfaces. Physical Review B, 1988, 38, 4033-4044.	3.2	127
170	Electronic band structure ofCaBi2Sr2Cu2O8. Physical Review Letters, 1988, 60, 1661-1664.	7.8	319
171	Monolayer growth and structure of ga on si(111). Physical Review B, 1988, 38, 7885-7888.	3.2	53
172	Model dielectric matrices for quasiparticle self-energy calculations. Physical Review B, 1988, 37, 2733-2736.	3.2	155
173	Geometric and Local Electronic Structure of Si(111)-As. Physical Review Letters, 1988, 60, 116-119.	7.8	124
174	Origin of the optical transitions in ordered Si/Ge(001) superlattices. Physical Review B, 1988, 37, 10195-10198.	3.2	46
175	The Self Energy Approach for Calculation of Quasiparticle Energies in Materials Systems. Materials Research Society Symposia Proceedings, 1988, 141, 79.	0.1	0
176	Theory of Optical Transitions in SinGen(001) Strained Layer Superlattices. Materials Research Society Symposia Proceedings, 1987, 102, 413.	0.1	3
177	Theory of optical transitions in Si/Ge(001) strained-layer superlattices. Physical Review B, 1987, 36, 9683-9693.	3.2	198
178	Many-body calculation of surface states: As on Ge(111). Physical Review Letters, 1987, 58, 1551-1554.	7.8	98
179	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.	3.2	62
180	Location of atoms in the first monolayer of GaAs on Si. Physical Review Letters, 1987, 59, 2180-2183.	7.8	53

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182	Ab initiostatic dielectric matrices from the density-functional approach. I. Formulation and application to semiconductors and insulators. Physical Review B, 1987, 35, 5585-5601.	3.2	338
183	Theory of quasiparticle energies: Band gaps and excitation spectra in solids. International Journal of Quantum Chemistry, 1987, 32, 31-44.	2.0	10
184	Electron correlation in semiconductors and insulators: Band gaps and quasiparticle energies. Physical Review B, 1986, 34, 5390-5413.	3.2	3,310
185	Spin-orbit splitting in semiconductors and insulators from theab initiopseudopotential. Physical Review B, 1986, 34, 2920-2922.	3.2	147
186	Electron correlation and the band gap in ionic crystals. Physical Review B, 1985, 32, 7005-7008.	3.2	97
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