Mark S Hybertsen

List of Publications by Citations

184 papers	25,122 citations	73 h-index	158 g-index
195 ext. papers	27,095 ext. citations	7.7 avg, IF	6.89 L-index

#	Paper	IF	Citations
184	Electron correlation in semiconductors and insulators: Band gaps and quasiparticle energies. *Physical Review B*, **1986**, 34, 5390-5413	3.3	2875
183	Exciton binding energy and nonhydrogenic Rydberg series in monolayer WS(2). *Physical Review Letters*, **2014**, 113, 076802	7.4	1358
182	Dependence of single-molecule junction conductance on molecular conformation. *Nature*, **2006**, 442, 904-7	50.4	1100
181	First-principles theory of quasiparticles: Calculation of band gaps in semiconductors and insulators. *Physical Review Letters*, **1985**, 55, 1418-1421	7.4	1096
180	Graphene oxidation: thickness-dependent etching and strong chemical doping. *Nano Letters*, **2008**, 8, 1965-70	11.5	704
179	Visualizing individual nitrogen dopants in monolayer graphene. *Science*, **2011**, 333, 999-1003	33.3	697
178	Renormalization of molecular electronic levels at metal-molecule interfaces. *Physical Review Letters* , **2006**, 97, 216405	7.4	693
177	Single-molecule circuits with well-defined molecular conductance. *Nano Letters*, **2006**, 6, 458-62	11.5	671
176	Calculation of Coulomb-interaction parameters for La2CuO4 using a constrained-density-functional approach. *Physical Review B*, **1989**, 39, 9028-9041	3.3	659
175	Theory of neutral and charged excitons in monolayer transition metal dichalcogenides. *Physical Review B*, **2013**, 88,	3.3	579
174	Mechanically controlled binary conductance switching of a single-molecule junction. *Nature Nanotechnology*, **2009**, 4, 230-4	28.7	515
173	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, 9209-12	11.5	494
172	Electronic states in La2-xSrxCuO4+ delta probed by soft-x-ray absorption. *Physical Review Letters*, **1991**, 66, 104-107	7.4	431
171	Renormalization from density-functional theory to strong-coupling models for electronic states in Cu-O materials. *Physical Review B*, **1990**, 41, 11068-11072	3.3	411
170	Amine-gold linked single-molecule circuits: experiment and theory. *Nano Letters*, **2007**, 7, 3477-82	11.5	403
169	Observation of biexcitons in monolayer WSe2. *Nature Physics*, **2015**, 11, 477-481	16.2	399
168	Connecting dopant bond type with electronic structure in N-doped graphene. *Nano Letters*, **2012**, 12, 4025-31	11.5	381

167	Absorption and emission of light in nanoscale silicon structures. *Physical Review Letters*, **1994**, 72, 1514-1517	7.4	350
166	Ab initio static dielectric matrices from the density-functional approach. I. Formulation and application to semiconductors and insulators. *Physical Review B*, **1987**, 35, 5585-5601	3.3	311
165	Electronic band structure of CaBi2Sr2Cu2O8. *Physical Review Letters*, **1988**, 60, 1661-1664	7.4	310
164	Contact chemistry and single-molecule conductance: a comparison of phosphines, methyl sulfides, and amines. *Journal of the American Chemical Society*, **2007**, 129, 15768-9	16.4	299
163	Electronics and chemistry: varying single-molecule junction conductance using chemical substituents. *Nano Letters*, **2007**, 7, 502-6	11.5	281
162	Microscopic theory of singlet exciton fission. II. Application to pentacene dimers and the role of superexchange. *Journal of Chemical Physics*, **2013**, 138, 114103	3.9	260
161	Observation of Excitonic Rydberg States in Monolayer MoS2 and WS2 by Photoluminescence Excitation Spectroscopy. *Nano Letters*, **2015**, 15, 2992-7	11.5	259
160	Probing the conductance superposition law in single-molecule circuits with parallel paths. *Nature Nanotechnology*, **2012**, 7, 663-7	28.7	258
159	Exciton condensate in semiconductor quantum well structures. *Physical Review Letters*, **1995**, 74, 1633-1636	7.4	243
158	The quantum coherent mechanism for singlet fission: experiment and theory. *Accounts of Chemical Research*, **2013**, 46, 1321-9	24.3	214
157	Tailoring the electronic structure in bilayer molybdenum disulfide via interlayer twist. *Nano Letters*, **2014**, 14, 3869-75	11.5	213
156	Structure and electronic properties of graphene nanoislands on Co(0001). *Nano Letters*, **2009**, 9, 2844-8	11.5	213
155	Interface structure between silicon and its oxide by first-principles molecular dynamics. *Nature*, **1998**, 396, 58-60	50.4	209
154	In situ formation of highly conducting covalent Au-C contacts for single-molecule junctions. *Nature Nanotechnology*, **2011**, 6, 353-7	28.7	206
153	Electronic structure of few-layer epitaxial graphene on Ru(0001). *Nano Letters*, **2009**, 9, 2654-60	11.5	203
152	Theory of Si 2p core-level shifts at the Si(001)-SiO2 interface. *Physical Review B*, **1996**, 53, 10942-10950	3.3	200
151	Formation and evolution of single-molecule junctions. *Physical Review Letters*, **2009**, 102, 126803	7.4	197
150	Theory of optical transitions in Si/Ge(001) strained-layer superlattices. *Physical Review B*, **1987**, 36, 9683-9693	3.9	191

149	Microscopic theory of singlet exciton fission. I. General formulation. *Journal of Chemical Physics*, **2013**, 138, 114102	3.9	182
148	Quasiparticle and optical properties of rutile and anatase TiO2. *Physical Review B*, **2010**, 82,	3.3	176
147	Si 2p core-level shifts at the Si(001)-SiO2 interface: A first-principles study. *Physical Review Letters*, **1995**, 74, 1024-1027	7.4	174
146	Local atomic and electronic structure of boron chemical doping in monolayer graphene. *Nano Letters*, **2013**, 13, 4659-65	11.5	168
145	Observation of graphene bubbles and effective mass transport under graphene films. *Nano Letters*, **2009**, 9, 332-7	11.5	164
144	Conductance and geometry of pyridine-linked single-molecule junctions. *Journal of the American Chemical Society*, **2010**, 132, 6817-21	16.4	160
143	Theory of quasiparticle energies in alkali metals. *Physical Review Letters*, **1987**, 59, 819-822	7.4	159
142	Van der Waals interactions at metal/organic interfaces at the single-molecule level. *Nature Materials*, **2012**, 11, 872-6	27	151
141	Highly conducting π-conjugated molecular junctions covalently bonded to gold electrodes. *Journal of the American Chemical Society*, **2011**, 133, 17160-3	16.4	149
140	Model dielectric matrices for quasiparticle self-energy calculations. *Physical Review B*, **1988**, 37, 2733-2736	3.3	149
139	Microscopic theory of singlet exciton fission. III. Crystalline pentacene. *Journal of Chemical Physics*, **2014**, 141, 074705	3.9	135
138	Many-body calculation of the surface-state energies for Si(111)2 x 1. *Physical Review Letters*, **1991**, 66, 500-503	7.4	126
137	Theory of quasiparticle surface states in semiconductor surfaces. *Physical Review B*, **1988**, 38, 4033-4044	3.3	125
136	Geometric and local electronic structure of Si(111)-As. *Physical Review Letters*, **1988**, 60, 116-119	7.4	120
135	Spin-orbit splitting in semiconductors and insulators from the ab initio pseudopotential. *Physical Review B*, **1986**, 34, 2920-2922	3.3	118
134	Model for low-energy electronic states probed by x-ray absorption in high-Tc cuprates. *Physical Review B*, **1992**, 45, 10032-10050	3.3	114
133	Mechanics and chemistry: single molecule bond rupture forces correlate with molecular backbone structure. *Nano Letters*, **2011**, 11, 1518-23	11.5	113
132	Length-dependent thermopower of highly conducting Au-C bonded single molecule junctions. *Nano Letters*, **2013**, 13, 2889-94	11.5	109

131	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, 3597-607	16.4	109
130	Structurally relaxed models of the Si(001)-SiO2 interface. *Applied Physics Letters*, **1996**, 68, 625-627	3.4	104
129	Absorption and luminescence studies of free-standing porous silicon films. *Physical Review B*, **1994**, 49, 5386-5397	3.3	101
128	Quantum cascade lasers without intersubband population inversion. *Physical Review Letters*, **1996**, 76, 411-414	7.4	99
127	Linker dependent bond rupture force measurements in single-molecule junctions. *Journal of the American Chemical Society*, **2012**, 134, 4003-6	16.4	96
126	Quasiparticle excitation spectrum for nearly-free-electron metals. *Physical Review B*, **1989**, 39, 8198-8208	3.3	96
125	First-principles analysis of electronic states in silicon nanoscale quantum wires. *Physical Review B*, **1993**, 48, 4608-4611	3.3	95
124	Many-body calculation of surface states: As on Ge(111). *Physical Review Letters*, **1987**, 58, 1551-1554	7.4	95
123	Electron correlation and the band gap in ionic crystals. *Physical Review B*, **1985**, 32, 7005-7008	3.3	95
122	Multiphonon relaxation slows singlet fission in crystalline hexacene. *Journal of the American Chemical Society*, **2014**, 136, 10654-60	16.4	92
121	Quasiparticle calculation of valence band offset of AlAs-GaAs(001). *Solid State Communications*, **1988**, 66, 585-588	1.6	88
120	Auger recombination of excitons in one-dimensional systems. *Physical Review B*, **2006**, 73,	3.3	87
119	Amine-linked single-molecule circuits: systematic trends across molecular families. *Journal of Physics Condensed Matter*, **2008**, 20, 374115	1.8	85
118	Core-level photoemission measurements of valence-band offsets in highly strained heterojunctions: Si-Ge system. *Physical Review B*, **1989**, 39, 1235-1241	3.3	81
117	Conductance of molecular junctions formed with silver electrodes. *Nano Letters*, **2013**, 13, 3358-64	11.5	77
116	Frustrated rotations in single-molecule junctions. *Journal of the American Chemical Society*, **2009**, 131, 10820-1	16.4	77
115	Scanning tunneling microscopy images of alkane derivatives on graphite: role of electronic effects. *Nano Letters*, **2008**, 8, 3160-5	11.5	77
114	Transition structure at the Si(100)-SiO2 interface. *Physical Review Letters*, **2003**, 90, 186101	7.4	77

113	Local empirical pseudopotential approach to the optical properties of Si/Ge superlattices. *Physical Review B*, **1989**, 39, 7974-7977	3.3	77
112	Nonlocal-density-functional approximation for exchange and correlation in semiconductors. *Physical Review B*, **1984**, 30, 5777-5790	3.3	75
111	Segregation of sublattice domains in nitrogen-doped graphene. *Journal of the American Chemical Society*, **2014**, 136, 1391-7	16.4	73
110	Photocatalytic Water Oxidation at the GaN (101 0)Water Interface. *Journal of Physical Chemistry C*, **2010**, 114, 13695-13704	3.8	72
109	Formation of catalytic metal-molecule contacts. *Science*, **2005**, 309, 591-4	33.3	68
108	Single-molecule junction conductance through diaminoacenes. *Journal of the American Chemical Society*, **2007**, 129, 6714-5	16.4	67
107	Forming aromatic hemispheres on transition-metal surfaces. *Angewandte Chemie - International Edition*, **2007**, 46, 7891-5	16.4	67
106	. *IEEE Journal of Selected Topics in Quantum Electronics*, **1995**, 1, 250-263	3.8	66
105	Band offset transitivity at the InGaAs/InAlAs/InP(001) heterointerfaces. *Applied Physics Letters*, **1991**, 58, 1759-1761	3.4	66
104	Binding energies and spatial structures of small carrier complexes in monolayer transition-metal dichalcogenides via diffusion Monte Carlo. *Physical Review B*, **2015**, 92,	3.3	64
103	First-principles approach to calculating energy level alignment at aqueous semiconductor interfaces. *Physical Review Letters*, **2014**, 113, 176802	7.4	64
102	Ab initio static 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	3.3	61
101	Structural and chemical trends in doped silicon nanocrystals: First-principles calculations. *Physical Review B*, **2005**, 71,	3.3	60
100	Evaluation of quasiparticle energies for semiconductors without inversion symmetry. *Physical Review B*, **1989**, 40, 3162-3168	3.3	58
99	Bright and dark singlet excitons via linear and two-photon spectroscopy in monolayer transition-metal dichalcogenides. *Physical Review B*, **2015**, 92,	3.3	54
98	Flicker Noise as a Probe of Electronic Interaction at Metal-Single Molecule Interfaces. *Nano Letters*, **2015**, 15, 4143-9	11.5	54
97	Role of interface strain in a lattice-matched heterostructure. *Physical Review Letters*, **1990**, 64, 555-558	7.4	53
96	Monolayer growth and structure of Ga on Si(111). *Physical Review B*, **1988**, 38, 7885-7888	3.3	52

95	Structure-Property Relationships in Atomic-Scale Junctions: Histograms and Beyond. *Accounts of Chemical Research*, **2016**, 49, 452-60	24.3	51
94	Negative differential resistance in transport through organic molecules on silicon. *Physical Review Letters*, **2007**, 98, 066807	7.4	50
93	Water Adsorption on the GaN (101 0) Nonpolar Surface. *Journal of Physical Chemistry C*, **2009**, 113, 3365-3868	3.3	48
92	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,	3.3	48
91	GW approach to Anderson model out of equilibrium: Coulomb blockade and false hysteresis in the I□V characteristics. *Physical Review B*, **2009**, 79,	3.3	47
90	Location of atoms in the first monolayer of GaAs on Si. *Physical Review Letters*, **1987**, 59, 2180-2183	7.4	47
89	40-Gb/s tandem electroabsorption modulator. *IEEE Photonics Technology Letters*, **2002**, 14, 27-29	2.2	46
88	Origin of the optical transitions in ordered Si/Ge(001) superlattices. *Physical Review B*, **1988**, 37, 10195-10198	3.3	45
87	Visualization of lithium-ion transport and phase evolution within and between manganese oxide nanorods. *Nature Communications*, **2017**, 8, 15400	17.4	44
86	Edge structures for nanoscale graphene islands on Co(0001) surfaces. *ACS Nano*, **2014**, 8, 5765-73	16.7	44
85	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	6.7	44
84	Quasiparticle band gaps for ultrathin GaAs/AlAs(001) superlattices. *Physical Review Letters*, **1989**, 63, 1495-1498	7.4	44
83	Phase diagram, structure, and electronic properties of (Ga1□Znx)(N1□Ox) solid solutions from DFT-based simulations. *Physical Review B*, **2011**, 83,	3.3	43
82	Atomistic Interrogation of B-N Co-dopant Structures and Their Electronic Effects in Graphene. *ACS Nano*, **2016**, 10, 6574-84	16.7	42
81	Simulation and characterization of the selective area growth process. *Applied Physics Letters*, **1999**, 74, 2617-2619	3.4	42
80	Measurement of voltage-dependent electronic transport across amine-linked single-molecular-wire junctions. *Nanotechnology*, **2009**, 20, 434009	3.4	39
79	Synchrotron x-ray microdiffraction diagnostics of multilayer optoelectronic devices. *Applied Physics Letters*, **1999**, 75, 100-102	3.4	39
78	Quasiparticle band offset at the (001) interface and band gaps in ultrathin superlattices of GaAs-AlAs heterojunctions. *Physical Review B*, **1990**, 41, 10058-10067	3.3	39

77	Spherosiloxane H8Si8O12 clusters on Si(001): First-principles calculation of Si 2p core-level shifts. *Physical Review B*, **1996**, 54, R2339-R2342	3.3	38
76	Computational investigation of structural and electronic properties of aqueous interfaces of GaN, ZnO, and a GaN/ZnO alloy. *Physical Chemistry Chemical Physics*, **2014**, 16, 12057-66	3.6	37
75	Enhanced static approximation to the electron self-energy operator for efficient calculation of quasiparticle energies. *Physical Review B*, **2010**, 82,	3.3	37
74	Frustrated ostwald ripening in self-assembled monolayers of cruciform pi-systems. *Langmuir*, **2006**, 22, 10003-8	4	36
73	Determination of the structure and geometry of N-heterocyclic carbenes on Au(111) using high-resolution spectroscopy. *Chemical Science*, **2019**, 10, 930-935	9.4	35
72	Semiconductor-Based Photoelectrochemical Water Splitting at the Limit of Very Wide Depletion Region. *Advanced Functional Materials*, **2016**, 26, 219-225	15.6	34
71	Reliable Formation of Single Molecule Junctions with Air-Stable Diphenylphosphine Linkers. *Journal of Physical Chemistry Letters*, **2010**, 1, 2114-2119	6.4	34
70	Performance of carbon nanotube-dispersed thin-film transistors. *Applied Physics Letters*, **2006**, 89, 143501	3.4	32
69	Calculation of the many body interaction parameters in the highTc compound La2CuO4. *Physica C: Superconductivity and Its Applications*, **1988**, 153-155, 1217-1218	1.3	32
68	Non-local density functional theory for the electronic and structural properties of semiconductors. *Solid State Communications*, **1984**, 51, 451-454	1.6	31
67	Role of p-doping profile and regrowth on the static characteristics of 1.3-/spl mu/m MQW InGaAsP-InP lasers: experiment and modeling. *IEEE Journal of Quantum Electronics*, **1999**, 35, 1515-1520	2	30
66	The electrical properties of biphenylenes. *Organic Letters*, **2010**, 12, 4114-7	6.2	27
65	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	3.8	26
64	Electron-hole system revisited: A variational quantum Monte Carlo study. *Physical Review B*, **1996**, 54, 13575-13580	3.3	26
63	Piezoreflectance study of short-period strained Si-Ge superlattices grown on (001) Ge. *Physical Review B*, **1991**, 44, 5955-5957	3.3	26
62	Density-Functional Study of Adsorption of Isocyanides on a Gold (111) Surface. *Journal of Physical Chemistry C*, **2008**, 112, 3314-3320	3.8	24
61	Graphite, Tubular PAHs, and the Diffuse Interstellar Bands. *Astrophysical Journal*, **2006**, 638, L105-L108	4.7	22
60	Controlled Growth of Ceria Nanoarrays on Anatase Titania Powder: A Bottom-up Physical Picture. *Nano Letters*, **2017**, 17, 348-354	11.5	21

59	Photoinduced Water Oxidation at the Aqueous GaN (101 0) Interface: Deprotonation Kinetics of the First Proton-Coupled Electron-Transfer Step. *ACS Catalysis*, **2015**, 5, 2317-2323	13.1	21
58	Simulation of semiconductor quantum well lasers. *IEEE Transactions on Electron Devices*, **2000**, 47, 1917-1925	2.5	21
57	Analysis of T0 in 1.3 μm multi-quantum-well and bulk active lasers. *Applied Physics Letters*, **1995**, 66, 2613-2615	3.4	21
56	Impedance-corrected carrier lifetime measurements in semiconductor lasers. *Applied Physics Letters*, **1995**, 67, 1506-1508	3.4	20
55	A Physical Model for Understanding the Activation of MoS Basal-Plane Sulfur Atoms for the Hydrogen Evolution Reaction. *Angewandte Chemie - International Edition*, **2020**, 59, 14835-14841	16.4	19
54	Growth and structural analysis of an ordered boron monolayer in Si(100). *Physical Review B*, **1992**, 46, 12861-12864	3.3	19
53	First-principles study of Si 2p core-level shifts at water and hydrogen covered Si(001)2×1 surfaces. *Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena*, **1996**, 14, 2809		18
52	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	3.3	18
51	Si 2p core-level shifts in small molecules: a first principles study. *Physica Scripta*, **1996**, T66, 118-120	2.6	17
50	Quantitative bond energetics in atomic-scale junctions. *ACS Nano*, **2014**, 8, 7522-30	16.7	16
49	Energetics of Lithium Insertion into Magnetite, Defective Magnetite, and Maghemite. *Chemistry of Materials*, **2018**, 30, 7922-7937	9.6	16
48	Chemisorption pathways and Si 2p 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	3.4	15
47	Theoretical study of trends in conductance for molecular junctions formed with armchair carbon nanotube electrodes. *Physical Review B*, **2007**, 76,	3.3	14
46	An Intrinsic Model for Radiative Recombination in Porous Silicon. *Materials Research Society Symposia Proceedings*, **1991**, 256, 179		14
45	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		14
44	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	1.3	13
43	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	3.8	12
42	Effect of p-doping on the temperature dependence of differential gain in FP and DFB 1.3-μm InGaAsP-InP multiple-quantum-well lasers. *IEEE Photonics Technology Letters*, **2000**, 12, 969-971	2.2	12

41	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	1.3	11
40	Charge localization and ordering in A2Mn8O16 hollandite group oxides: Impact of density functional theory approaches. *Physical Review Materials*, **2017**, 1,	3.2	11
39	Atomic Scale Account of the Surface Effect on Ionic Transport in Silver Hollandite. *Chemistry of Materials*, **2018**, 30, 6124-6133	9.6	10
38	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	3.8	9
37	Multiwavelength DFB laser array with integrated spot size converters. *IEEE Journal of Quantum Electronics*, **2000**, 36, 641-648	2	9
36	Design of medium band gap Ag-Bi-Nb-O and Ag-Bi-Ta-O semiconductors for driving direct water splitting with visible light. *Inorganic Chemistry*, **2013**, 52, 9192-205	5.1	8
35	Solvent Effects on the Self-Assembly of 1-Bromoeicosane on Graphite. Part II. Theory. *Journal of Physical Chemistry C*, **2009**, 113, 3641-3649	3.8	8
34	Microscopic simulation of the temperature dependence of static and dynamic 1.3-μm multi-quantum-well laser performance. *IEEE Journal of Quantum Electronics*, **2003**, 39, 120-129	2	8
33	Quantum beats in photon echo from four-waving mixing. *Physical Review Letters*, **1994**, 73, 209	7.4	8
32	The Atomic and Electronic Structure of Ordered Buried B(2x1) Layers in Si(100). *Materials Science Forum*, **1992**, 83-87, 1391-1396	0.4	8
31	Modeling single molecule junction mechanics as a probe of interface bonding. *Journal of Chemical Physics*, **2017**, 146, 092323	3.9	7
30	Charge disproportionation in tetragonal La2MoO5, a small band gap semiconductor influenced by direct Mo-Mo bonding. *Journal of the American Chemical Society*, **2015**, 137, 1245-57	16.4	7
29	Four-wave mixing and terahertz emission from three-level systems in quantum wells: Effects of inhomogeneous broadening. *Physical Review B*, **1994**, 50, 11915-11923	3.3	7
28	Microscopic theory of heterojunction band offsets. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **1992**, 14, 254-261	3.1	7
27	Theory of quasiparticle energies: Band gaps and excitation spectra in solids. *International Journal of Quantum Chemistry*, **1987**, 32, 31-44	2.1	7
26	Microscopic relaxation channels in materials for superconducting qubits. *Communications Materials*, **2021**, 2,	6	7
25	Ultrathin Amorphous Titania on Nanowires: Optimization of Conformal Growth and Elucidation of Atomic-Scale Motifs. *Nano Letters*, **2019**, 19, 3457-3463	11.5	6
24	Self-Energy Approach to Quasiparticle Energies Using a Density Functional Treatment of Dielectric Screening. *Advances in Quantum Chemistry*, **1990**, 155-174	1.4	6

23	Description of quasiparticle and satellite properties via cumulant expansions of the retarded one-particle Green's function. *Physical Review B*, **2016**, 94,	3.3	6
22	Observation of intercalation-driven zone folding in quasi-free-standing graphene energy bands. *Physical Review B*, **2019**, 99,	3.3	5
21	Excitation and characterization of image potential state electrons on quasi-free-standing graphene. *Physical Review B*, **2018**, 97,	3.3	5
20	Silicon crystal distortions at the Si(1 0 0)/SiO2 interface from analysis of ion-scattering. *Microelectronic Engineering*, **2004**, 72, 197-200	2.5	5
19	Core-Level Shifts in Si(001)-SiO2 Systems: The Value of First-Principle Investigations **1998**, 89-102		5
18	Piezoreflectance of strained Si/Ge superlattices grown on Ge(001). *Surface Science*, **1992**, 267, 99-102	1.8	4
17	Probing Structural Reconstruction of Metal Nanoparticles under Annealing and Water Vapor Conditions: A Theoretical Study. *Journal of Physical Chemistry C*, **2019**, 123, 29783-29793	3.8	4
16	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	9.6	4
15	A Physical Model for Understanding the Activation of MoS2 Basal-Plane Sulfur Atoms for the Hydrogen Evolution Reaction. *Angewandte Chemie*, **2020**, 132, 14945-14951	3.6	3
14	Excitons in atomically thin transition-metal dichalcogenides **2014**,		3
13	Effects of the interfacial polarization on tunneling in surface coupled quantum dots. *Physical Review B*, **2012**, 86,	3.3	3
12	Theory of the Quasiparticle Effective Masses in Semiconductors Based on an Electron Self Energy Approach. *Materials Research Society Symposia Proceedings*, **1990**, 193, 113		3
11	Theory of Optical Transitions in SinGen(001) Strained Layer Superlattices. *Materials Research Society Symposia Proceedings*, **1987**, 102, 413		3
10	Ion scattering simulations of the Si(100)/SiO2 interface. *Physical Review B*, **2006**, 74,	3.3	2
9	Renormalization from Density Functional Theory to Strong Coupling Models for the Electronic Structure of La2CuO4. *Materials Research Society Symposia Proceedings*, **1989**, 169, 19		0
8	Hydrogen bonded trimesic acid networks on Cu(111) reveal how basic chemical properties are imprinted in HR-AFM images. *Nanoscale*, **2021**, 13, 18473-18482	7.7	0
7	Simultaneous Measurement of Force and Conductance Across Single Molecule Junctions. *Conference Proceedings of the Society for Experimental Mechanics*, **2013**, 75-84	0.3	
6	Auger Recombination of Excitons in Semiconducting Carbon Nanotubes. *Springer Series in Chemical Physics*, **2007**, 683-685	0.3	

5 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

4 The Self Energy Approach for Calculation of Quasiparticle Energies in Materials Systems. *Materials Research Society Symposia Proceedings*, **1988**, 141, 79

3 Models for the Electronic Structure of Cuprates. *Physics and Chemistry of Materials With Low-dimensional Structures*, **1992**, 229-245

2 Microscopic Theory of the Properties of Semiconductor Heterojunctions. *Kluwer International Series in Engineering and Computer Science*, **1996**, 189-200

1 In-situ Probe of Lithium-ion Transport and Phase Evolution Within and Between Silver Hollandite Nanorods. *Microscopy and Microanalysis*, **2018**, 24, 1516-1517 0.5