Kristian S Thygesen

List of Publications by Citations

201 papers	15,949 citations	61 h-index	121 g-index
213 ext. papers	18,430 ext. citations	7 avg, IF	7.2 L-index

#	Paper	IF	Citations
201	The atomic simulation environment-a Python library for working with atoms. *Journal of Physics Condensed Matter*, **2017**, 29, 273002	1.8	1097
200	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. *Journal of Physics Condensed Matter*, **2010**, 22, 253202	1.8	1092
199	Phonon-limited mobility in n-type single-layer MoS2 from first principles. *Physical Review B*, **2012**, 85,	3.3	847
198	Computational 2D Materials Database: Electronic Structure of Transition-Metal Dichalcogenides and Oxides. *Journal of Physical Chemistry C*, **2015**, 119, 13169-13183	3.8	615
197	Electrical conductivity in Li2O2 and its role in determining capacity limitations in non-aqueous Li-O2 batteries. *Journal of Chemical Physics*, **2011**, 135, 214704	3.9	460
196	Observation of quantum interference in molecular charge transport. *Nature Nanotechnology*, **2012**, 7, 305-9	28.7	404
195	The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals. *2D Materials*, **2018**, 5, 042002	5.9	399
194	Graphene on metals: A van der Waals density functional study. *Physical Review B*, **2010**, 81,	3.3	397
193	Communications: Elementary oxygen electrode reactions in the aprotic Li-air battery. *Journal of Chemical Physics*, **2010**, 132, 071101	3.9	319
192	Computational screening of perovskite metal oxides for optimal solar light capture. *Energy and Environmental Science*, **2012**, 5, 5814-5819	35.4	301
191	The relation between structure and quantum interference in single molecule junctions. *Nano Letters*, **2010**, 10, 4260-5	11.5	255
190	Localized atomic basis set in the projector augmented wave method. *Physical Review B*, **2009**, 80,	3.3	232
189	Electrochemical CO2 and CO Reduction on Metal-Functionalized Porphyrin-like Graphene. *Journal of Physical Chemistry C*, **2013**, 117, 9187-9195	3.8	218
188	Fully self-consistent GW calculations for molecules. *Physical Review B*, **2010**, 81,	3.3	205
187	Acoustic phonon limited mobility in two-dimensional semiconductors: Deformation potential and piezoelectric scattering in monolayer MoS2 from first principles. *Physical Review B*, **2013**, 87,	3.3	195
186	Polarization-induced renormalization of molecular levels at metallic and semiconducting surfaces. *Physical Review B*, **2009**, 80,	3.3	195
185	Finite Size Effects in Chemical Bonding: From Small Clusters to Solids. *Catalysis Letters*, **2011**, 141, 1067-1071	2.8	193

184	Conserving GW scheme for nonequilibrium quantum transport in molecular contacts. *Physical Review B*, **2008**, 77,	3.3	190
183	New cubic perovskites for one- and two-photon water splitting using the computational materials repository. *Energy and Environmental Science*, **2012**, 5, 9034	35.4	178
182	How dielectric screening in two-dimensional crystals affects the convergence of excited-state calculations: Monolayer MoS2. *Physical Review B*, **2013**, 88,	3.3	174
181	Bandgap calculations and trends of organometal halide perovskites. *APL Materials*, **2014**, 2, 081514	5.7	167
180	Self-consistent GW calculations of electronic transport in thiol- and amine-linked molecular junctions. *Physical Review B*, **2011**, 83,	3.3	165
179	Excitons in van der Waals heterostructures: The important role of dielectric screening. *Physical Review B*, **2015**, 92,	3.3	159
178	Dispersive and covalent interactions between graphene and metal surfaces from the random phase approximation. *Physical Review Letters*, **2011**, 107, 156401	7.4	158
177	Renormalization of molecular quasiparticle levels at metal-molecule interfaces: trends across binding regimes. *Physical Review Letters*, **2009**, 102, 046802	7.4	158
176	Stretching dependence of the vibration modes of a single-molecule Pt–H2–Pt bridge. *Physical Review B*, **2005**, 71,	3.3	135
175	Calculating excitons, plasmons, and quasiparticles in 2D materials and van der Waals heterostructures. *2D Materials*, **2017**, 4, 022004	5.9	131
174	Interlayer Excitons and Band Alignment in MoS/hBN/WSe van der Waals Heterostructures. *Nano Letters*, **2017**, 17, 938-945	11.5	131
173	Simple Screened Hydrogen Model of Excitons in Two-Dimensional Materials. *Physical Review Letters* , **2016**, 116, 056401	7.4	131
172	Quasiparticle GW calculations for solids, molecules, and two-dimensional materials. *Physical Review B*, **2013**, 87,	3.3	130
171	DFT+U Study of Polaronic Conduction in Li2O2 and Li2CO3: Implications for Li–Air Batteries. *Journal of Physical Chemistry C*, **2013**, 117, 5568-5577	3.8	127
170	Dielectric Genome of van der Waals Heterostructures. *Nano Letters*, **2015**, 15, 4616-21	11.5	125
169	Two-Dimensional MXenes as Catalysts for Electrochemical Hydrogen Evolution: A Computational Screening Study. *Journal of Physical Chemistry C*, **2017**, 121, 13593-13598	3.8	115
168	Molecular transport calculations with Wannier functions. *Chemical Physics*, **2005**, 319, 111-125	2.3	111
167	Random phase approximation applied to solids, molecules, and graphene-metal interfaces: From van der Waals to covalent bonding. *Physical Review B*, **2013**, 87,	3.3	109

166	Linear density response function in the projector augmented wave method: Applications to solids, surfaces, and interfaces. *Physical Review B*, **2011**, 83,	3.3	107
165	Influence of functional groups on charge transport in molecular junctions. *Journal of Chemical Physics*, **2008**, 128, 111103	3.9	107
164	New Light-Harvesting Materials Using Accurate and Efficient Bandgap Calculations. *Advanced Energy Materials*, **2015**, 5, 1400915	21.8	105
163	Cross-conjugation and quantum interference: a general correlation?. *Physical Chemistry Chemical Physics*, **2014**, 16, 653-62	3.6	101
162	Benchmark density functional theory calculations for nanoscale conductance. *Journal of Chemical Physics*, **2008**, 128, 114714	3.9	99
161	Electrochemical control of single-molecule conductance by Fermi-level tuning and conjugation switching. *Journal of the American Chemical Society*, **2014**, 136, 17922-5	16.4	95
160	Nonequilibrium GW approach to quantum transport in nano-scale contacts. *Journal of Chemical Physics*, **2007**, 126, 091101	3.9	95
159	Stability and Electronic Properties of TiO2 Nanostructures With and Without B and N Doping. *Journal of Physical Chemistry C*, **2009**, 113, 12301-12308	3.8	94
158	Unraveling the acoustic electron-phonon interaction in graphene. *Physical Review B*, **2012**, 85,	3.3	91
157	Electrochemical control of quantum interference in anthraquinone-based molecular switches. *Journal of Chemical Physics*, **2010**, 132, 224104	3.9	90
156	Renormalization of optical excitations in molecules near a metal surface. *Physical Review Letters*, **2011**, 106, 187402	7.4	87
155	Defect-Tolerant Monolayer Transition Metal Dichalcogenides. *Nano Letters*, **2016**, 16, 2234-9	11.5	86
154	The role of transition metal interfaces on the electronic transport in lithium□air batteries. *Catalysis Today*, **2011**, 165, 2-9	5.3	82
153	Band Gap Tuning and Defect Tolerance of Atomically Thin Two-Dimensional Organic-Inorganic Halide Perovskites. *Journal of Physical Chemistry Letters*, **2016**, 7, 4346-4352	6.4	78
152	Tuning the Schottky Barrier at the Graphene/MoS2 Interface by Electron Doping: Density Functional Theory and Many-Body Calculations. *Journal of Physical Chemistry C*, **2015**, 119, 19928-19933	3.8	76
151	Dissociation of two-dimensional excitons in monolayer WSe. *Nature Communications*, **2018**, 9, 1633	17.4	76
150	Density functional theory based screening of ternary alkali-transition metal borohydrides: a computational material design project. *Journal of Chemical Physics*, **2009**, 131, 014101	3.9	74
149	Four-atom period in the conductance of monatomic Al wires. *Physical Review Letters*, **2003**, 91, 146801	7.4	73

148	Machine learning-based screening of complex molecules for polymer solar cells. *Journal of Chemical Physics*, **2018**, 148, 241735	3.9	71
147	Impact of exchange-correlation effects on the IV characteristics of a molecular junction. *Physical Review Letters*, **2008**, 100, 166804	7.4	71
146	Nonlocal screening of plasmons in graphene by semiconducting and metallic substrates: first-principles calculations. *Physical Review Letters*, **2011**, 106, 146803	7.4	69
145	Engineering covalently bonded 2D layered materials by self-intercalation. *Nature*, **2020**, 581, 171-177	50.4	68
144	Conductance calculations with a wavelet basis set. *Physical Review B*, **2003**, 67,	3.3	66
143	Two-Dimensional Metal Dichalcogenides and Oxides for Hydrogen Evolution: A Computational Screening Approach. *Journal of Physical Chemistry Letters*, **2015**, 6, 1577-85	6.4	64
142	Graphical prediction of quantum interference-induced transmission nodes in functionalized organic molecules. *Physical Chemistry Chemical Physics*, **2011**, 13, 14311-7	3.6	62
141	Sulfide perovskites for solar energy conversion applications: computational screening and synthesis of the selected compound LaYS3. *Energy and Environmental Science*, **2017**, 10, 2579-2593	35.4	61
140	Conduction mechanism in a molecular hydrogen contact. *Physical Review Letters*, **2005**, 94, 036807	7.4	60
139	Electron transport through an interacting region: The case of a nonorthogonal basis set. *Physical Review B*, **2006**, 73,	3.3	59
138	Forces and conductances in a single-molecule bipyridine junction. *Physical Review B*, **2005**, 72,	3.3	59
137	Quantifying transition voltage spectroscopy of molecular junctions: Ab initio calculations. *Physical Review B*, **2010**, 82,	3.3	57
136	High oscillator strength interlayer excitons in two-dimensional heterostructures for mid-infrared photodetection. *Nature Nanotechnology*, **2020**, 15, 675-682	28.7	56
135	Layered van der Waals crystals with hyperbolic light dispersion. *Nature Communications*, **2017**, 8, 320	17.4	56
134	Extending the random-phase approximation for electronic correlation energies: The renormalized adiabatic local density approximation. *Physical Review B*, **2012**, 86,	3.3	56
133	Partly occupied Wannier functions. *Physical Review Letters*, **2005**, 94, 026405	7.4	56
132	Band structure engineering in van der Waals heterostructures via dielectric screening: the GW method. *2D Materials*, **2017**, 4, 025059	5.9	55
131	Multiterminal single-molecule graphene-nanoribbon junctions with the thermoelectric figure of merit optimized via evanescent mode transport and gate voltage. *Physical Review B*, **2011**, 84,	3.3	55

130	Single-molecule electrochemical transistor utilizing a nickel-pyridyl spinterface. *Nano Letters*, **2015**, 15, 275-80	11.5	54
129	High throughput computational screening for 2D ferromagnetic materials: the critical role of anisotropy and local correlations. *2D Materials*, **2019**, 6, 045018	5.9	53
128	Influence of O2 and N2 on the conductivity of carbon nanotube networks. *Physical Review B*, **2009**, 79,	3.3	53
127	Anharmonic stabilization and band gap renormalization in the perovskite CsSnI3. *Physical Review B*, **2015**, 92,	3.3	52
126	First-principles study of surface plasmons on Ag(111) and H/Ag(111). *Physical Review B*, **2011**, 84,	3.3	52
125	Efficient many-body calculations for two-dimensional materials using exact limits for the screened potential: Band gaps of MoS2, h-BN, and phosphorene. *Physical Review B*, **2016**, 94,	3.3	52
124	Finite-momentum exciton landscape in mono- and bilayer transition metal dichalcogenides. *2D Materials*, **2019**, 6, 035003	5.9	51
123	First-principles quantum transport modeling of thermoelectricity in single-molecule nanojunctions with graphene nanoribbon electrodes. *Journal of Computational Electronics*, **2012**, 11, 78-92	1.8	50
122	Stability and bandgaps of layered perovskites for one- and two-photon water splitting. *New Journal of Physics*, **2013**, 15, 105026	2.9	49
121	Plasmonic eigenmodes in individual and bow-tie graphene nanotriangles. *Scientific Reports*, **2015**, 5, 9535	4.9	48
120	Conductance of Conjugated Molecular Wires: Length Dependence, Anchoring Groups, and Band Alignment. *Journal of Physical Chemistry C*, **2009**, 113, 20967-20973	3.8	48
119	Fundamental limitation of electrocatalytic methane conversion to methanol. *Physical Chemistry Chemical Physics*, **2018**, 20, 11152-11159	3.6	47
118	Accurate Ground-State Energies of Solids and Molecules from Time-Dependent Density-Functional Theory. *Physical Review Letters*, **2014**, 112,	7.4	47
117	Avoiding pitfalls in the modeling of electrochemical interfaces. *Chemical Physics Letters*, **2013**, 555, 145-148	2.3	47
116	Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces. *Journal of Physical Chemistry C*, **2011**, 115, 2244-2252	3.8	46
115	Nano-imaging of intersubband transitions in van der Waals quantum wells. *Nature Nanotechnology*, **2018**, 13, 1035-1041	28.7	45
114	Beyond the random phase approximation: Improved description of short-range correlation by a renormalized adiabatic local density approximation. *Physical Review B*, **2013**, 88,	3.3	45
113	Stacked Janus Device Concepts: Abrupt pn-Junctions and Cross-Plane Channels. *Nano Letters*, **2018**, 18, 7275-7281	11.5	45

112	Adiabatic-connection fluctuation-dissipation DFT for the structural properties of solids-The renormalized ALDA and electron gas kernels. *Journal of Chemical Physics*, **2015**, 143, 102802	3.9	44
111	Communication: strong excitonic and vibronic effects determine the optical properties of Li2O2. *Journal of Chemical Physics*, **2011**, 135, 121101	3.9	44
110	Dark excitations in monolayer transition metal dichalcogenides. *Physical Review B*, **2017**, 96,	3.3	44
109	Efficient Charge Separation in 2D Janus van der Waals Structures with Built-in Electric Fields and Intrinsic p□ Doping. *Journal of Physical Chemistry C*, **2018**, 122, 24520-24526	3.8	44
108	Interlayer Excitons with Large Optical Amplitudes in Layered van der Waals Materials. *Nano Letters*, **2018**, 18, 2984-2989	11.5	43
107	Classifying the Electronic and Optical Properties of Janus Monolayers. *ACS Nano*, **2019**, 13, 13354-13364	16.7	43
106	Probing the local nature of excitons and plasmons in few-layer MoS2. *Npj 2D Materials and Applications*, **2017**, 1,	8.8	41
105	Interference and k-point sampling in the supercell approach to phase-coherent transport. *Physical Review B*, **2005**, 72,	3.3	41
104	Interlayer Trions in the MoS/WS van der Waals Heterostructure. *Nano Letters*, **2018**, 18, 1460-1465	11.5	40
103	Calculated Pourbaix Diagrams of Cubic Perovskites for Water Splitting: Stability Against Corrosion. *Topics in Catalysis*, **2014**, 57, 265-272	2.3	40
102	Optical properties of bulk semiconductors and graphene/boron nitride: The Bethe-Salpeter equation with derivative discontinuity-corrected density functional energies. *Physical Review B*, **2012**, 86,	3.3	40
101	Visualizing hybridized quantum plasmons in coupled nanowires: From classical to tunneling regime. *Physical Review B*, **2013**, 87,	3.3	40
100	Electronic shell structure and chemisorption on gold nanoparticles. *Physical Review B*, **2011**, 84,	3.3	40
99	Band structure engineered layered metals for low-loss plasmonics. *Nature Communications*, **2017**, 8, 15133	17.4	39
98	Conventional and acoustic surface plasmons on noble metal surfaces: A time-dependent density functional theory study. *Physical Review B*, **2012**, 86,	3.3	39
97	Direct measurement and modulation of single-molecule coordinative bonding forces in a transition metal complex. *Nature Communications*, **2013**, 4, 2121	17.4	38
96	Conductance of sidewall-functionalized carbon nanotubes: universal dependence on adsorption sites. *Physical Review Letters*, **2008**, 101, 236806	7.4	38
95	Discovering two-dimensional topological insulators from high-throughput computations. *Physical Review Materials*, **2019**, 3,	3.2	38

94	Temperature effects on quantum interference in molecular junctions. *Physical Review B*, **2014**, 89,	3.3	37
93	Stark shift and electric-field-induced dissociation of excitons in monolayer MoS2 and hBN/MoS2 heterostructures. *Physical Review B*, **2016**, 94,	3.3	36
92	Controlling Electrical Conductance through a Conjugated Cruciform Molecule by Selective Anchoring to Gold Electrodes. *Angewandte Chemie - International Edition*, **2015**, 54, 14304-7	16.4	35
91	Plasmons in metallic monolayer and bilayer transition metal dichalcogenides. *Physical Review B*, **2013**, 88,	3.3	35
90	Towards quantitative accuracy in first-principles transport calculations: The GW method applied to alkane/gold junctions. *Beilstein Journal of Nanotechnology*, **2011**, 2, 746-54	3	35
89	Modeling nanoscale gas sensors under realistic conditions: Computational screening of metal-doped carbon nanotubes. *Physical Review B*, **2010**, 81,	3.3	33
88	Recent progress of the computational 2D materials database (C2DB). *2D Materials*, **2021**, 8, 044002	5.9	33
87	Benchmark Database of Transition Metal Surface and Adsorption Energies from Many-Body Perturbation Theory. *Journal of Physical Chemistry C*, **2018**, 122, 4381-4390	3.8	32
86	Computational screening of functionalized zinc porphyrins for dye sensitized solar cells. *Physical Chemistry Chemical Physics*, **2013**, 15, 19478-86	3.6	32
85	Comparative study of anchoring groups for molecular electronics: structure and conductance of Au-S-Au and Au-NH(2)-Au junctions. *Journal of Physics Condensed Matter*, **2008**, 20, 374101	1.8	32
84	High-Throughput Computational Assessment of Previously Synthesized Semiconductors for Photovoltaic and Photoelectrochemical Devices. *ACS Energy Letters*, **2018**, 3, 436-446	20.1	31
83	Spatially resolved quantum plasmon modes in metallic nano-films from first-principles. *Physical Review B*, **2012**, 86,	3.3	31
82	Static correlation beyond the random phase approximation: dissociating H2 with the Bethe-Salpeter equation and time-dependent GW. *Journal of Chemical Physics*, **2014**, 140, 164116	3.9	30
81	Ab initio nonequilibrium quantum transport and forces with the real-space projector augmented wave method. *Physical Review B*, **2012**, 85,	3.3	30
80	Energy level alignment and quantum conductance of functionalized metal-molecule junctions: density functional theory versus GW calculations. *Journal of Chemical Physics*, **2013**, 139, 184307	3.9	30
79	Calculated optical absorption of different perovskite phases. *Journal of Materials Chemistry A*, **2015**, 3, 12343-12349	13	29
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77	Plasmons on the edge of MoS2 nanostructures. *Physical Review B*, **2014**, 90,	3.3	29

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75	Partly occupied Wannier functions: Construction and applications. *Physical Review B*, **2005**, 72,	3.3	29
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72	Exciton ionization in multilayer transition-metal dichalcogenides. *New Journal of Physics*, **2016**, 18, 073043	3.3	27
71	Benchmarking GW against exact diagonalization for semiempirical models. *Physical Review B*, **2010**, 81,	3.3	27
70	Magnetoresistance and negative differential resistance in Ni/graphene/Ni vertical heterostructures driven by finite bias voltage: A first-principles study. *Physical Review B*, **2012**, 85,	3.3	26
69	Improving transition voltage spectroscopy of molecular junctions. *Physical Review B*, **2011**, 83,	3.3	26
68	Electron transport in a Pt□OPt nanocontact: Density functional theory calculations. *Physical Review B*, **2006**, 73,	3.3	26
67	Simple vertex correction improves GW band energies of bulk and two-dimensional crystals. *Physical Review B*, **2017**, 96,	3.3	25
66	Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM) Electrostatic Embedding and Application to a Solvated Diplatinum Complex. *Journal of Chemical Theory and Computation*, **2017**, 13, 6010-6022	6.4	24
65	Image-charge-induced localization of molecular orbitals at metal-molecule interfaces: Self-consistent GW calculations. *Physical Review B*, **2012**, 86,	3.3	23
64	Strain sensitivity of band gaps of Sn-containing semiconductors. *Physical Review B*, **2015**, 91,	3.3	22
63	Anab initiostudy of electron transport through nitrobenzene: the influence of leads and contacts. *Nanotechnology*, **2005**, 16, S155-S160	3.4	22
62	Local Plasmon Engineering in Doped Graphene. *ACS Nano*, **2018**, 12, 1837-1848	16.7	21
61	Inelastic scattering in metal-H2-metal junctions. *Physical Review B*, **2009**, 79,	3.3	21
60	Robust conductance of dumbbell molecular junctions with fullerene anchoring groups. *Journal of Chemical Physics*, **2011**, 135, 144104	3.9	20
59	MyQueue: Task and workflow scheduling system. *Journal of Open Source Software*, **2020**, 5, 1844	5.2	20

58	Spin-dependent electron-phonon coupling in the valence band of single-layer WS2. *Physical Review B*, **2017**, 96,	3.3	19
57	Beyond the RPA and GW methods with adiabatic xc-kernels for accurate ground state and quasiparticle energies. *Npj Computational Materials*, **2019**, 5,	10.9	19
56	VNCB defect as source of single photon emission from hexagonal boron nitride. *2D Materials*, **2020**, 7, 031007	5.9	18
55	Electron□phonon interaction and transport properties of metallic bulk and monolayer transition metal dichalcogenide TaS 2. *2D Materials*, **2018**, 5, 015009	5.9	18
54	A library of ab initio Raman spectra for automated identification of 2D materials. *Nature Communications*, **2020**, 11, 3011	17.4	17
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52	Hot-electron-assisted femtochemistry at surfaces: A time-dependent density functional theory approach. *Physical Review B*, **2009**, 79,	3.3	17
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50	Importance of the Reorganization Energy Barrier in Computational Design of Porphyrin-Based Solar Cells with Cobalt-Based Redox Mediators. *Journal of Physical Chemistry C*, **2015**, 119, 12792-12800	3.8	16
49	Hubbard-U corrected Hamiltonians for non-self-consistent random-phase approximation total-energy calculations: A study of ZnS, TiO2, and NiO. *Physical Review B*, **2016**, 93,	3.3	15
48	Improved description of metal oxide stability: Beyond the random phase approximation with renormalized kernels. *Physical Review B*, **2015**, 92,	3.3	15
47	Dynamical image-charge effect in molecular tunnel junctions: Beyond energy level alignment. *Physical Review B*, **2014**, 89,	3.3	15
46	Atomically Thin Ordered Alloys of Transition Metal Dichalcogenides: Stability and Band Structures. *Journal of Physical Chemistry C*, **2016**, 120, 23024-23029	3.8	14
45	Quantum conductance of 4,4-bipyridine molecular junctions: Role of electrode work function and local d band. *Physical Review B*, **2008**, 78,	3.3	14
44	Limitations of effective medium theory in multilayer graphite/hBN heterostructures. *Physical Review B*, **2016**, 94,	3.3	13
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41	Edge effects on optically detected magnetic resonance of vacancy defects in hexagonal boron nitride. *Communications Physics*, **2020**, 3,	5.4	13

40	Tunable free-electron X-ray radiation from van der Waals materials. *Nature Photonics*, **2020**, 14, 686-692	33.9	13
39	Efficient Ab Initio Modeling of Dielectric Screening in 2D van der Waals Materials: Including Phonons, Substrates, and Doping. *Journal of Physical Chemistry C*, **2020**, 124, 11609-11616	3.8	12
38	Electrical tuning of optically active interlayer excitons in bilayer MoS. *Nature Nanotechnology*, **2021**, 16, 888-893	28.7	12
37	Controlled generation of luminescent centers in hexagonal boron nitride by irradiation engineering. *Science Advances*, **2021**, 7,	14.3	12
36	Effect of edge plasmons on the optical properties of MoS2 monolayer flakes. *Physical Review B*, **2017**, 96,	3.3	11
35	Bandgap Engineering of Double Perovskites for One- and Two-photon Water Splitting. *Materials Research Society Symposia Proceedings*, **2013**, 1523, 601		11
34	Band structure of MoSTe Janus nanotubes. *Physical Review Materials*, **2021**, 5,	3.2	11
33	First-principles modelling of scanning tunneling microscopy using non-equilibrium Green functions. *Frontiers of Physics in China*, **2010**, 5, 369-379		10
32	Two-Dimensional Materials with Giant Optical Nonlinearities near the Theoretical Upper Limit. *ACS Nano*, **2021**, 15, 7155-7167	16.7	10
31	Strong Plasmon-Phonon Splitting and Hybridization in 2D Materials Revealed through a Self-Energy Approach. *ACS Photonics*, **2017**, 4, 2908-2915	6.3	9
30	A Protocol for Fast Prediction of Electronic and Optical Properties of Donor-Acceptor Polymers Using Density Functional Theory and the Tight-Binding Method. *Journal of Physical Chemistry A*, **2019**, 123, 4980-4989	2.8	9
29	Design of two-photon molecular tandem architectures for solar cells by theory. *Chemical Science*, **2015**, 6, 3018-3025	9.4	9
28	Unraveling the not-so-large trion binding energy in monolayer black phosphorus. *2D Materials*, **2018**, 5, 041007	5.9	9
27	Structural and chemical mechanisms governing stability of inorganic Janus nanotubes. *Npj Computational Materials*, **2021**, 7,	10.9	9
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25	Conductance of quantum spin Hall edge states from first principles: The critical role of magnetic impurities and inter-edge scattering. *Physical Review B*, **2020**, 101,	3.3	8
24	Band-gap engineering of functional perovskites through quantum confinement and tunneling. *Physical Review B*, **2015**, 91,	3.3	8
23	Designing multifunctional chemical sensors using Ni and Cu doped carbon nanotubes. *Physica Status Solidi (B): Basic Research*, **2010**, 247, 2678-2682	1.3	8

22	Intrinsic Defects in MoS Grown by Pulsed Laser Deposition: From Monolayers to Bilayers. *ACS Nano*, **2021**, 15, 2858-2868	16.7	8
21	Atomic Simulation Recipes A Python framework and library for automated workflows. *Computational Materials Science*, **2021**, 199, 110731	3.2	8
20	Reply to comment on The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals *2D Materials*, **2019**, 6, 048002	5.9	7
19	Electrically controlled dielectric band gap engineering in a two-dimensional semiconductor. *Physical Review B*, **2020**, 101,	3.3	7
18	Publisher's Note: Polarization-induced renormalization of molecular levels at metallic and semiconducting surfaces [Phys. Rev. B 80, 245427 (2009)]. *Physical Review B*, **2010**, 81,	3.3	7
17	Controlling Electrical Conductance through a Conjugated Cruciform Molecule by Selective Anchoring to Gold Electrodes. *Angewandte Chemie*, **2015**, 127, 14512-14515	3.6	6
16	Anisotropic properties of monolayer 2D materials: An overview from the C2DB database. *Journal of Applied Physics*, **2020**, 128, 105101	2.5	6
15	Role of Long-Range Dispersion Forces in Modeling of MXenes as Battery Electrode Materials. *Journal of Physical Chemistry C*, **2019**, 123, 4064-4071	3.8	5
14	Engineering Atomically Sharp Potential Steps and Band Alignment at Solid Interfaces using 2D Janus Layers. *Journal of Physical Chemistry C*, **2020**, 124, 9572-9580	3.8	5
13	Simultaneous description of conductance and thermopower in single-molecule junctions from many-body ab initio calculations. *Physical Review B*, **2014**, 90,	3.3	5
12	Emergent scale invariance of nonclassical plasmons in graphene nanoribbons. *Physical Review B*, **2018**, 98,	3.3	5
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