Kristian S Thygesen

List of Publications by Year
in descending order

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206 papers	21,206 citations	11608 70 h-index	10127 140 g-index
213 all docs	213 docs citations	213 times ranked	20662 citing authors

#	Article	IF	Citations
1	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	0.7	1,933
2	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	0.7	1,451
3	Phonon-limited mobility in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-type single-layer MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>from first principles. Physical Review B, 2012, 85, .	1.1	1,033
4	Computational 2D Materials Database: Electronic Structure of Transition-Metal Dichalcogenides and Oxides. Journal of Physical Chemistry C, 2015, 119, 13169-13183.	1.5	902
5	The Computational 2D Materials Database: high-throughput modeling and discovery of atomically thin crystals. 2D Materials, 2018, 5, 042002.	2.0	711
6	Electrical conductivity in Li2O2 and its role in determining capacity limitations in non-aqueous Li-O2 batteries. Journal of Chemical Physics, 2011, 135, 214704.	1.2	502
7	Observation of quantum interference in molecular charge transport. Nature Nanotechnology, 2012, 7, 305-309.	15.6	465
8	Graphene on metals: A van der Waals density functional study. Physical Review B, 2010, 81, .	1.1	431
9	Communications: Elementary oxygen electrode reactions in the aprotic Li-air battery. Journal of Chemical Physics, 2010, 132, 071101.	1.2	367
10	Computational screening of perovskite metal oxides for optimal solar light capture. Energy and Environmental Science, 2012, 5, 5814-5819.	15.6	354
11	Localized atomic basis set in the projector augmented wave method. Physical Review B, 2009, 80, .	1.1	297
12	The Relation between Structure and Quantum Interference in Single Molecule Junctions. Nano Letters, 2010, 10, 4260-4265.	4.5	296
13	Electrochemical CO₂ and CO Reduction on Metal-Functionalized Porphyrin-like Graphene. Journal of Physical Chemistry C, 2013, 117, 9187-9195.	1.5	260
14	Acoustic phonon limited mobility in two-dimensional semiconductors: Deformation potential and piezoelectric scattering in monolayer MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>from first principles. Physical Review B, 2013, 87, .	1.1	243
15	Finite Size Effects in Chemical Bonding: From Small Clusters to Solids. Catalysis Letters, 2011, 141, 1067-1071.	1.4	234
16	How dielectric screening in two-dimensional crystals affects the convergence of excited-state calculations: Monolayer MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 88, .	1.1	226
17	Fully self-consistent GW calculations for molecules. Physical Review B, 2010, 81, .	1.1	225
18	Bandgap calculations and trends of organometal halide perovskites. APL Materials, 2014, 2, .	2.2	222

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19	Recent progress of the Computational 2D Materials Database (C2DB). 2D Materials, 2021, 8, 044002.	2.0	218
20	Polarization-induced renormalization of molecular levels at metallic and semiconducting surfaces. Physical Review B, 2009, 80, .	1.1	214
21	New cubic perovskites for one- and two-photon water splitting using the computational materials repository. Energy and Environmental Science, 2012, 5, 9034.	15.6	211
22	Excitons in van der Waals heterostructures: The important role of dielectric screening. Physical Review B, 2015, 92, .	1.1	211
23	Conserving<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>scheme for nonequilibrium quantum transport in molecular contacts. Physical Review B, 2008, 77, .	1.1	204
24	Calculating excitons, plasmons, and quasiparticles in 2D materials and van der Waals heterostructures. 2D Materials, 2017, 4, 022004.	2.0	189
25	Self-consistent GW calculations of electronic transport in thiol- and amine-linked molecular junctions. Physical Review B, 2011, 83, .	1.1	186
26	Engineering covalently bonded 2D layered materials by self-intercalation. Nature, 2020, 581, 171-177.	13.7	185
27	Two-Dimensional MXenes as Catalysts for Electrochemical Hydrogen Evolution: A Computational Screening Study. Journal of Physical Chemistry C, 2017, 121, 13593-13598.	1.5	183
28	Interlayer Excitons and Band Alignment in MoS₂/hBN/WSe₂ van der Waals Heterostructures. Nano Letters, 2017, 17, 938-945.	4.5	174
29	Renormalization of Molecular Quasiparticle Levels at Metal-Molecule Interfaces: Trends across Binding Regimes. Physical Review Letters, 2009, 102, 046802.	2.9	173
30	Dielectric Genome of van der Waals Heterostructures. Nano Letters, 2015, 15, 4616-4621.	4.5	173
31	Dispersive and Covalent Interactions between Graphene and Metal Surfaces from the Random Phase Approximation. Physical Review Letters, 2011, 107, 156401.	2.9	172
32	Quasiparticle GW calculations for solids, molecules, and two-dimensional materials. Physical Review B, 2013, 87, .	1.1	168
33	Simple Screened Hydrogen Model of Excitons in Two-Dimensional Materials. Physical Review Letters, 2016, 116, 056401.	2.9	167
34	Stretching dependence of the vibration modes of a single-moleculePtâˆ’H2âˆ’Ptbridge. Physical Review B, 2005, 71, .	1.1	142
35	Linear density response function in the projector augmented wave method: Applications to solids, surfaces, and interfaces. Physical Review B, 2011, 83, .	1.1	142
36	DFT+U Study of Polaronic Conduction in Li₂O₂ and Li₂CO₃: Implications for Liâ€“Air Batteries. Journal of Physical Chemistry C, 2013, 117, 5568-5577.	1.5	142

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37	High oscillator strength interlayer excitons in two-dimensional heterostructures for mid-infrared photodetection. Nature Nanotechnology, 2020, 15, 675-682.	15.6	129
38	New Lightâ€Harvesting Materials Using Accurate and Efficient Bandgap Calculations. Advanced Energy Materials, 2015, 5, 1400915.	10.2	124
39	Unraveling the acoustic electron-phonon interaction in graphene. Physical Review B, 2012, 85, .	1.1	122
40	Molecular transport calculations with Wannier functions. Chemical Physics, 2005, 319, 111-125.	0.9	120
41	Random phase approximation applied to solids, molecules, and graphene-metal interfaces: From van der Waals to covalent bonding. Physical Review B, 2013, 87, .	1.1	120
42	Electrochemical Control of Single-Molecule Conductance by Fermi-Level Tuning and Conjugation Switching. Journal of the American Chemical Society, 2014, 136, 17922-17925.	6.6	119
43	Cross-conjugation and quantum interference: a general correlation?. Physical Chemistry Chemical Physics, 2014, 16, 653-662.	1.3	116
44	Dissociation of two-dimensional excitons in monolayer WSe2. Nature Communications, 2018, 9, 1633.	5.8	116
45	Influence of functional groups on charge transport in molecular junctions. Journal of Chemical Physics, 2008, 128, 111103.	1.2	114
46	Defect-Tolerant Monolayer Transition Metal Dichalcogenides. Nano Letters, 2016, 16, 2234-2239.	4.5	111
47	Benchmark density functional theory calculations for nanoscale conductance. Journal of Chemical Physics, 2008, 128, 114714.	1.2	109
48	Band Gap Tuning and Defect Tolerance of Atomically Thin Two-Dimensional Organicâ€“Inorganic Halide Perovskites. Journal of Physical Chemistry Letters, 2016, 7, 4346-4352.	2.1	107
49	Stability and Electronic Properties of TiO₂ Nanostructures With and Without B and N Doping. Journal of Physical Chemistry C, 2009, 113, 12301-12308.	1.5	102
50	Nonequilibrium GW approach to quantum transport in nano-scale contacts. Journal of Chemical Physics, 2007, 126, 091101.	1.2	100
51	Electrochemical control of quantum interference in anthraquinone-based molecular switches. Journal of Chemical Physics, 2010, 132, 224104.	1.2	98
52	Renormalization of Optical Excitations in Molecules near a Metal Surface. Physical Review Letters, 2011, 106, 187402.	2.9	98
53	Machine learning-based screening of complex molecules for polymer solar cells. Journal of Chemical Physics, 2018, 148, 241735.	1.2	94
54	Classifying the Electronic and Optical Properties of Janus Monolayers. ACS Nano, 2019, 13, 13354-13364.	7.3	93

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55	Sulfide perovskites for solar energy conversion applications: computational screening and synthesis of the selected compound LaYS₃. Energy and Environmental Science, 2017, 10, 2579-2593.	15.6	91
56	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.	1.5	89
57	High throughput computational screening for 2D ferromagnetic materials: the critical role of anisotropy and local correlations. 2D Materials, 2019, 6, 045018.	2.0	89
58	The role of transition metal interfaces on the electronic transport in lithiumâ€“air batteries. Catalysis Today, 2011, 165, 2-9.	2.2	87
59	Finite-momentum exciton landscape in mono- and bilayer transition metal dichalcogenides. 2D Materials, 2019, 6, 035003.	2.0	84
60	Four-Atom Period in the Conductance of Monatomic Al Wires. Physical Review Letters, 2003, 91, 146801.	2.9	82
61	Stacked Janus Device Concepts: Abrupt pn-Junctions and Cross-Plane Channels. Nano Letters, 2018, 18, 7275-7281.	4.5	82
62	Impact of Exchange-Correlation Effects on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>I</mml:mi><mml:mi>V</mml:mi></mml:math>Characteristics of a Molecular Junction. Physical Review Letters, 2008, 100, 166804.	2.9	79
63	Layered van der Waals crystals with hyperbolic light dispersion. Nature Communications, 2017, 8, 320.	5.8	79
64	Efficient Charge Separation in 2D Janus van der Waals Structures with Built-in Electric Fields and Intrinsic pâ€“n Doping. Journal of Physical Chemistry C, 2018, 122, 24520-24526.	1.5	79
65	Density functional theory based screening of ternary alkali-transition metal borohydrides: A computational material design project. Journal of Chemical Physics, 2009, 131, 014101.	1.2	77
66	Anharmonic stabilization and band gap renormalization in the perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CsSnI</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2015, 92, .	1.1	76
67	Efficient many-body calculations for two-dimensional materials using exact limits for the screened potential: Band gaps of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">MoS</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo>,</mml:mo><mml:mo>Â</mml:mo><mml:mi>h</m and phosphorene. Physical Review B, 2016, 94, .	1.1	76
68	Two-Dimensional Metal Dichalcogenides and Oxides for Hydrogen Evolution: A Computational Screening Approach. Journal of Physical Chemistry Letters, 2015, 6, 1577-1585.	2.1	75
69	Nano-imaging of intersubband transitions in van der Waals quantum wells. Nature Nanotechnology, 2018, 13, 1035-1041.	15.6	75
70	Conductance calculations with a wavelet basis set. Physical Review B, 2003, 67, .	1.1	74
71	Nonlocal Screening of Plasmons in Graphene by Semiconducting and Metallic Substrates: First-Principles Calculations. Physical Review Letters, 2011, 106, 146803.	2.9	73
72	Single-Molecule Electrochemical Transistor Utilizing a Nickel-Pyridyl Spinterface. Nano Letters, 2015, 15, 275-280.	4.5	73

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73	Fundamental limitation of electrocatalytic methane conversion to methanol. Physical Chemistry Chemical Physics, 2018, 20, 11152-11159.	1.3	73
74	Graphical prediction of quantum interference-induced transmission nodes in functionalized organic molecules. Physical Chemistry Chemical Physics, 2011, 13, 14311.	1.3	71
75	Band structure engineering in van der Waals heterostructures via dielectric screening: the GÎ”W method. 2D Materials, 2017, 4, 025059.	2.0	71
76	Interlayer Excitons with Large Optical Amplitudes in Layered van der Waals Materials. Nano Letters, 2018, 18, 2984-2989.	4.5	71
77	Multiterminal single-moleculeâ€“graphene-nanoribbon junctions with the thermoelectric figure of merit optimized via evanescent mode transport and gate voltage. Physical Review B, 2011, 84, .	1.1	69
78	Forces and conductances in a single-molecule bipyridine junction. Physical Review B, 2005, 72, .	1.1	65
79	Partly Occupied Wannier Functions. Physical Review Letters, 2005, 94, 026405.	2.9	64
80	Electron transport through an interacting region: The case of a nonorthogonal basis set. Physical Review B, 2006, 73, .	1.1	64
81	First-principles study of surface plasmons on Ag(111) and H/Ag(111). Physical Review B, 2011, 84, .	1.1	64
82	Conduction Mechanism in a Molecular Hydrogen Contact. Physical Review Letters, 2005, 94, 036807.	2.9	63
83	Plasmonic eigenmodes in individual and bow-tie graphene nanotriangles. Scientific Reports, 2015, 5, 9535.	1.6	62
84	Extending the random-phase approximation for electronic correlation energies: The renormalized adiabatic local density approximation. Physical Review B, 2012, 86, .	1.1	61
85	Quantifying transition voltage spectroscopy of molecular junctions:Ab initiocalculations. Physical Review B, 2010, 82, .	1.1	60
86	Electrical tuning of optically active interlayer excitons in bilayer MoS2. Nature Nanotechnology, 2021, 16, 888-893.	15.6	60
87	Dark excitations in monolayer transition metal dichalcogenides. Physical Review B, 2017, 96, .	1.1	60
88	Discovering two-dimensional topological insulators from high-throughput computations. Physical Review Materials, 2019, 3, .	0.9	60
89	Band structure engineered layered metals for low-loss plasmonics. Nature Communications, 2017, 8, 15133.	5.8	59
90	Probing the local nature of excitons and plasmons in few-layer MoS2. Npj 2D Materials and Applications, 2017, 1, .	3.9	58

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91	First-principles quantum transport modeling of thermoelectricity in single-molecule nanojunctions with graphene nanoribbon electrodes. Journal of Computational Electronics, 2012, 11, 78-92.	1.3	57
92	Adiabatic-connection fluctuation-dissipation DFT for the structural properties of solidsâ€"The renormalized ALDA and electron gas kernels. Journal of Chemical Physics, 2015, 143, 102802.	1.2	56
93	Interlayer Trions in the MoS₂/WS₂ van der Waals Heterostructure. Nano Letters, 2018, 18, 1460-1465.	4.5	56
94	Influence ofO2andN2on the conductivity of carbon nanotube networks. Physical Review B, 2009, 79, .	1.1	55
95	Accurate Ground-State Energies of Solids and Molecules from Time-Dependent Density-Functional Theory. Physical Review Letters, 2014, 112, .	2.9	53
96	Benchmark Database of Transition Metal Surface and Adsorption Energies from Many-Body Perturbation Theory. Journal of Physical Chemistry C, 2018, 122, 4381-4390.	1.5	53
97	Conductance of Conjugated Molecular Wires: Length Dependence, Anchoring Groups, and Band Alignment. Journal of Physical Chemistry C, 2009, 113, 20967-20973.	1.5	52
98	Trends in Metal Oxide Stability for Nanorods, Nanotubes, and Surfaces. Journal of Physical Chemistry C, 2011, 115, 2244-2252.	1.5	52
99	V_NC_B defect as source of single photon emission from hexagonal boron nitride. 2D Materials, 2020, 7, 031007.	2.0	52
100	Conventional and acoustic surface plasmons on noble metal surfaces: A time-dependent density functional theory study. Physical Review B, 2012, 86, .	1.1	51
101	Stability and bandgaps of layered perovskites for one- and two-photon water splitting. New Journal of Physics, 2013, 15, 105026.	1.2	51
102	High-Throughput Computational Assessment of Previously Synthesized Semiconductors for Photovoltaic and Photoelectrochemical Devices. ACS Energy Letters, 2018, 3, 436-446.	8.8	51
103	Controlled generation of luminescent centers in hexagonal boron nitride by irradiation engineering. Science Advances, 2021, 7, .	4.7	51
104	Beyond the random phase approximation: Improved description of short-range correlation by a renormalized adiabatic local density approximation. Physical Review B, 2013, 88, .	1.1	50
105	Avoiding pitfalls in the modeling of electrochemical interfaces. Chemical Physics Letters, 2013, 555, 145-148.	1.2	50
106	Tunable free-electron X-ray radiation from van der Waals materials. Nature Photonics, 2020, 14, 686-692.	15.6	48
107	Interference andk-point sampling in the supercell approach to phase-coherent transport. Physical Review B, 2005, 72, .	1.1	47
108	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, .	1.1	47

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109	Calculated Pourbaix Diagrams of Cubic Perovskites for Water Splitting: Stability Against Corrosion. Topics in Catalysis, 2014, 57, 265-272.	1.3	47
110	Stark shift and electric-field-induced dissociation of excitons in monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="bold">MoS</mml:mi><mml:mn mathvariant="bold">2</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>h</mml:mi><mml:mrow><mml:mi mathvariant="bold">BN</mml:mi><mml:mo>/</mml:mo><mml:msub><mml:mi mathvariant="bold">MoS<	1.1	47
111	Communication: Strong excitonic and vibronic effects determine the optical properties of Li2O2. Journal of Chemical Physics, 2011, 135, 121101.	1.2	45
112	Electronic shell structure and chemisorption on gold nanoparticles. Physical Review B, 2011, 84, .	1.1	44
113	Direct measurement and modulation of single-molecule coordinative bonding forces in a transition metal complex. Nature Communications, 2013, 4, 2121.	5.8	43
114	Plasmons in metallic monolayer and bilayer transition metal dichalcogenides. Physical Review B, 2013, 88, .	1.1	43
115	A library of ab initio Raman spectra for automated identification of 2D materials. Nature Communications, 2020, 11, 3011.	5.8	43
116	Conductance of Sidewall-Functionalized Carbon Nanotubes: Universal Dependence on Adsorption Sites. Physical Review Letters, 2008, 101, 236806.	2.9	41
117	Visualizing hybridized quantum plasmons in coupled nanowires: From classical to tunneling regime. Physical Review B, 2013, 87, .	1.1	41
118	Temperature effects on quantum interference in molecular junctions. Physical Review B, 2014, 89, .	1.1	40
119	Controlling Electrical Conductance through a Ï€â€Conjugated Cruciform Molecule by Selective Anchoring to Gold Electrodes. Angewandte Chemie - International Edition, 2015, 54, 14304-14307.	7.2	40
120	Intrinsic Defects in MoS₂ Grown by Pulsed Laser Deposition: From Monolayers to Bilayers. ACS Nano, 2021, 15, 2858-2868.	7.3	40
121	Exciton ionization in multilayer transition-metal dichalcogenides. New Journal of Physics, 2016, 18, 073043.	1.2	39
122	Partly occupied Wannier functions: Construction and applications. Physical Review B, 2005, 72, .	1.1	38
123	Modeling nanoscale gas sensors under realistic conditions: Computational screening of metal-doped carbon nanotubes. Physical Review B, 2010, 81, .	1.1	37
124	Simple vertex correction improves <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m band energies of bulk and two-dimensional crystals. Physical Review B, 2017, 96, .	1.1	37
125	Towards quantitative accuracy in first-principles transport calculations: The GW method applied to alkane/gold junctions. Beilstein Journal of Nanotechnology, 2011, 2, 746-754.	1.5	36
126	Spatially resolved quantum plasmon modes in metallic nano-films from first-principles. Physical Review B, 2012, 86, .	1.1	36

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127	Computational screening of functionalized zinc porphyrins for dye sensitized solar cells. Physical Chemistry Chemical Physics, 2013, 15, 19478.	1.3	36
128	Plasmons on the edge of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">MoS</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>nanostructures. Physical Review B, 2014, 90, .	1.1	36
129	MyQueue: Task and workflow scheduling system. Journal of Open Source Software, 2020, 5, 1844.	2.0	36
130	Energy level alignment and quantum conductance of functionalized metal-molecule junctions: Density functional theory versus GW calculations. Journal of Chemical Physics, 2013, 139, 184307.	1.2	35
131	Calculated optical absorption of different perovskite phases. Journal of Materials Chemistry A, 2015, 3, 12343-12349.	5.2	35
132	Making the most of materials computations. Science, 2016, 354, 180-181.	6.0	35
133	Finite Bias Calculations to Model Interface Dipoles in Electrochemical Cells at the Atomic Scale. Journal of Physical Chemistry C, 2016, 120, 13485-13491.	1.5	35
134	Atomic Simulation Recipes: A Python framework and library for automated workflows. Computational Materials Science, 2021, 199, 110731.	1.4	35
135	Comparative study of anchoring groups for molecular electronics: structure and conductance of Auâ€“Sâ€“Au and Auâ€“NH2â€“Au junctions. Journal of Physics Condensed Matter, 2008, 20, 374101.	0.7	34
136	First-principles calculations of graphene nanoribbons in gaseous environments: Structural and electronic properties. Physical Review B, 2010, 82, .	1.1	33
137	Ab initiononequilibrium quantum transport and forces with the real-space projector augmented wave method. Physical Review B, 2012, 85, .	1.1	33
138	Beyond the RPA and GW methods with adiabatic xc-kernels for accurate ground state and quasiparticle energies. Npj Computational Materials, 2019, 5, .	3.5	33
139	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.	1.2	32
140	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.	2.3	32
141	Quantum point defects in 2D materials - the QPOD database. Npj Computational Materials, 2022, 8, .	3.5	30
142	Improving transition voltage spectroscopy of molecular junctions. Physical Review B, 2011, 83, .	1.1	29
143	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, .	1.1	29
144	Optimizing porphyrins for dye sensitized solar cells using large-scale ab initio calculations. Physical Chemistry Chemical Physics, 2014, 16, 16246-16254.	1.3	29

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145	Electronâ€“phonon interaction and transport properties of metallic bulk and monolayer transition metal dichalcogenide TaS ₂. 2D Materials, 2018, 5, 015009.	2.0	29
146	Two-Dimensional Materials with Giant Optical Nonlinearities near the Theoretical Upper Limit. ACS Nano, 2021, 15, 7155-7167.	7.3	29
147	Electron transport in aPtâ^'COâ^'Ptnanocontact: Density functional theory calculations. Physical Review B, 2006, 73, .	1.1	28
148	Edge effects on optically detected magnetic resonance of vacancy defects in hexagonal boron nitride. Communications Physics, 2020, 3, .	2.0	28
149	Benchmarking GW against exact diagonalization for semiempirical models. Physical Review B, 2010, 81, .	1.1	27
150	Image-charge-induced localization of molecular orbitals at metal-molecule interfaces: Self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculations. Physical Review B, 2012, 86, .	1.1	26
151	Enhancing and Controlling Plasmons in Janus MoSSeâ€“Graphene Based van der Waals Heterostructures. Journal of Physical Chemistry C, 2019, 123, 16373-16379.	1.5	26
152	Local Plasmon Engineering in Doped Graphene. ACS Nano, 2018, 12, 1837-1848.	7.3	25
153	Representing individual electronic states for machine learning GW band structures of 2D materials. Nature Communications, 2022, 13, 468.	5.8	25
154	Strain sensitivity of band gaps of Sn-containing semiconductors. Physical Review B, 2015, 91, .	1.1	24
155	Anab initiostudy of electron transport through nitrobenzene: the influence of leads and contacts. Nanotechnology, 2005, 16, S155-S160.	1.3	23
156	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.	1.5	23
157	Band structure of MoSTe Janus nanotubes. Physical Review Materials, 2021, 5, .	0.9	23
158	Quantitatively accurate calculations of conductance and thermopower of molecular junctions. Physica Status Solidi (B): Basic Research, 2013, 250, 2394-2402.	0.7	22
159	Spin-dependent electron-phonon coupling in the valence band of single-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2017, 96, .	1.1	22
160	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.	1.5	22
161	Structural and chemical mechanisms governing stability of inorganic Janus nanotubes. Npj Computational Materials, 2021, 7, .	3.5	22
162	Inelastic scattering in metal-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> junctions. Physical Review B, 2009, 79, .	1.1	21

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163	Robust conductance of dumbbell molecular junctions with fullerene anchoring groups. Journal of Chemical Physics, 2011, 135, 144104.	1.2	21
164	Effect of edge plasmons on the optical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml monolayer flakes. Physical Review B, 2017, 96, .	1.1	21
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