

Richard G Hennig

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/9543004/publications.pdf>

Version: 2024-02-01

160
papers

14,027
citations

24978

57
h-index

20307

116
g-index

169
all docs

169
docs citations

169
times ranked

17227
citing authors

#	ARTICLE	IF	CITATIONS
1	Implicit solvation model for density-functional study of nanocrystal surfaces and reaction pathways. Journal of Chemical Physics, 2014, 140, 084106.	1.2	1,676
2	Single-Layer Group-III Monochalcogenide Photocatalysts for Water Splitting. Chemistry of Materials, 2013, 25, 3232-3238.	3.2	675
3	Computational Screening of 2D Materials for Photocatalysis. Journal of Physical Chemistry Letters, 2015, 6, 1087-1098.	2.1	641
4	Implicit self-consistent electrolyte model in plane-wave density-functional theory. Journal of Chemical Physics, 2019, 151, 234101.	1.2	561
5	Computational Search for Single-Layer Transition-Metal Dichalcogenide Photocatalysts. Journal of Physical Chemistry C, 2013, 117, 20440-20445.	1.5	468
6	<i>Ab Initio</i> Prediction of Piezoelectricity in Two-Dimensional Materials. ACS Nano, 2015, 9, 9885-9891.	7.3	445
7	Alleviation of the Fermion-Sign Problem by Optimization of Many-Body Wave Functions. Physical Review Letters, 2007, 98, 110201.	2.9	411
8	Computational discovery of single-layer III-V materials. Physical Review B, 2013, 87, .	1.1	318
9	Softened Elastic Response and Unzipping in Chemical Vapor Deposition Graphene Membranes. Nano Letters, 2011, 11, 2259-2263.	4.5	316
10	Angle-Resolved Raman Imaging of Interlayer Rotations and Interactions in Twisted Bilayer Graphene. Nano Letters, 2012, 12, 3162-3167.	4.5	299
11	Strong anisotropy and magnetostriction in the two-dimensional Stoner ferromagnet Fe_3X_2 . Physical Review B, 2016, 93, .	7.3	299
12	Enhanced Li^+ Batteries Using Amine-Functionalized Carbon Nanotubes in the Cathode. ACS Nano, 2016, 10, 1050-1059.	7.3	289
13	Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials. Physical Review Letters, 2017, 118, 106101.	2.9	262
14	Computational prediction of two-dimensional group-IV mono-chalcogenides. Applied Physics Letters, 2014, 105, .	1.5	245
15	Predicting Nanocrystal Shape through Consideration of Surface-Ligand Interactions. ACS Nano, 2012, 6, 2118-2127.	7.3	236
16	Theoretical perspective of photocatalytic properties of single-layer SnS_2 . Physical Review B, 2013, 88, .	1.1	215
17	van der Waals Epitaxial Growth of Graphene on Sapphire by Chemical Vapor Deposition without a Metal Catalyst. ACS Nano, 2013, 7, 385-395.	7.3	211
18	Accuracy of exchange-correlation functionals and effect of solvation on the surface energy of copper. Physical Review B, 2013, 87, .	1.1	211

#	ARTICLE	IF	CITATIONS
19	Impurities block the \pm to $\bar{\Gamma}$ martensitic transformation in titanium. Nature Materials, 2005, 4, 129-133.	13.3	207
20	Controlling Nanocrystal Superlattice Symmetry and Shape-Anisotropic Interactions through Variable Ligand Surface Coverage. Journal of the American Chemical Society, 2011, 133, 3131-3138.	6.6	198
21	Predicted Surface Composition and Thermodynamic Stability of MXenes in Solution. Journal of Physical Chemistry C, 2016, 120, 3550-3556.	1.5	196
22	Strong spin-lattice coupling in CrSiTe ₃ . APL Materials, 2015, 3, .	2.2	192
23	Stability and magnetism of strongly correlated single-layer VS_2 . Physical Review B, 2016, 93, .	1.1	173
24	Classical potential describes martensitic phase transformations between the \pm and $\bar{\Gamma}$ titanium phases. Physical Review B, 2008, 78, .	1.1	173
25	Two-Dimensional Intrinsic Half-Metals With Large Spin Gaps. Nano Letters, 2017, 17, 5251-5257.	4.5	172
26	New Mechanism for the \pm to $\bar{\Gamma}$ Martensitic Transformation in Pure Titanium. Physical Review Letters, 2003, 91, 025701.	2.9	156
27	Solid-Solid Phase Transformations Induced through Cation Exchange and Strain in 2D Heterostructured Copper Sulfide Nanocrystals. Nano Letters, 2014, 14, 7090-7099.	4.5	147
28	ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials. Physical Chemistry Chemical Physics, 2015, 17, 3383-3393.	1.3	143
29	The structural evolution and diffusion during the chemical transformation from cobalt to cobalt phosphide nanoparticles. Journal of Materials Chemistry, 2011, 21, 11498.	6.7	136
30	Comparison of screened hybrid density functional theory to diffusion Monte Carlo in calculations of total energies of silicon phases and defects. Physical Review B, 2006, 74, .	1.1	131
31	Synthesis of borophane polymorphs through hydrogenation of borophene. Science, 2021, 371, 1143-1148.	6.0	129
32	The Oxidation of Cobalt Nanoparticles into Kirkendall-Hollowed Co ₃ O ₄ : The Diffusion Mechanisms and Atomic Structural Transformations. Journal of Physical Chemistry C, 2013, 117, 14303-14312.	1.5	128
33	Hybrid cathode architectures for lithium batteries based on TiS ₂ and sulfur. Journal of Materials Chemistry A, 2015, 3, 19857-19866.	5.2	119
34	Three-Dimensionally Isotropic Negative Refractive Index Materials from Block Copolymer Self-Assembled Chiral Gyroid Networks. Angewandte Chemie - International Edition, 2011, 50, 11985-11989.	7.2	116
35	Electronic structures of single-layer boron pnictides. Applied Physics Letters, 2012, 101, .	1.5	114
36	Ab initio synthesis of single-layer III-V materials. Physical Review B, 2014, 89, .	1.1	112

#	ARTICLE	IF	CITATIONS
37	Emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys. <i>Nature</i> , 2008, 451, 445-448.	13.7	111
38	Computational prediction and characterization of single-layer CrS ₂ . <i>Applied Physics Letters</i> , 2014, 104, 022116.	1.5	108
39	Density functional theory study of the electrochemical interface between a Pt electrode and an aqueous electrolyte using an implicit solvent method. <i>Journal of Chemical Physics</i> , 2015, 142, 234107.	1.2	103
40	MPInterfaces: A Materials Project based Python tool for high-throughput computational screening of interfacial systems. <i>Computational Materials Science</i> , 2016, 122, 183-190.	1.4	95
41	Computational Study of Low Interlayer Friction in Ti _n C _n (n = 1, 2, and 3) MXene. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 34467-34479.	4.0	93
42	Theoretical Studies of Carbonyl-Based Organic Molecules for Energy Storage Applications: The Heteroatom and Substituent Effect. <i>Journal of Physical Chemistry C</i> , 2014, 118, 6046-6051.	1.5	91
43	Dynamic instabilities in strongly correlated VSe_2 monolayers and bilayers. <i>Physical Review B</i> , 2017, 96, .		
44	Unintended Phosphorus Doping of Nickel Nanoparticles during Synthesis with TOP: A Discovery through Structural Analysis. <i>Nano Letters</i> , 2012, 12, 4530-4539.	4.5	81
45	Computational characterization of lightweight multilayer MXene Li-ion battery anodes. <i>Applied Physics Letters</i> , 2016, 108, .	1.5	79
46	The 2021 room-temperature superconductivity roadmap. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 183002.	0.7	79
47	Li-Carboxylate Anode Structure-Property Relationships from Molecular Modeling. <i>Chemistry of Materials</i> , 2013, 25, 132-141.	3.2	75
48	Computational discovery of stable M_2X_2 . <i>Physical Review B</i> , 2016, 94, .		
49	<i>Ab initio</i> based empirical potential used to study the mechanical properties of molybdenum. <i>Physical Review B</i> , 2012, 85, .	1.1	71
50	Complexity of Small Silicon Self-Interstitial Defects. <i>Physical Review Letters</i> , 2004, 92, 045501.	2.9	69
51	Tethered Molecular Sorbents: Enabling Metal-Sulfur Battery Cathodes. <i>Advanced Energy Materials</i> , 2014, 4, 1400390.	10.2	67
52	Phase transformation in Si from semiconducting diamond to metallic I^2-Sn phase in QMC and DFT under hydrostatic and anisotropic stress. <i>Physical Review B</i> , 2010, 82, .	1.1	65
53	Questioning the existence of a unique ground-state structure for Si clusters. <i>Physical Review B</i> , 2007, 75, .	1.1	62
54	Doping-controlled phase transitions in single-layer MoS_2 . <i>Physical Review B</i> , 2017, 96, .	1.1	62

#	ARTICLE	IF	CITATIONS
55	Rashba effect in single-layer antimony telluroiodide SbTeI. <i>Physical Review B</i> , 2015, 92, .	1.1	60
56	Computational discovery and characterization of polymorphic two-dimensional IV-V materials. <i>Applied Physics Letters</i> , 2016, 109, .	1.5	60
57	Grand-canonical evolutionary algorithm for the prediction of two-dimensional materials. <i>Physical Review B</i> , 2016, 93, .	1.1	59
58	Tailored redox functionality of small organics for pseudocapacitive electrodes. <i>Energy and Environmental Science</i> , 2012, 5, 7176.	15.6	58
59	Computational methods for 2D materials: discovery, property characterization, and application design. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 473001.	0.7	55
60	Computational identification of single-layer CdO for electronic and optical applications. <i>Applied Physics Letters</i> , 2013, 103, .	1.5	52
61	A grand canonical genetic algorithm for the prediction of multi-component phase diagrams and testing of empirical potentials. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 495401.	0.7	52
62	Structure of the icosahedral Ti-Zr-Ni quasicrystal. <i>Physical Review B</i> , 2003, 67, .	1.1	46
63	Computational synthesis of single-layer GaN on refractory materials. <i>Applied Physics Letters</i> , 2014, 105, .	1.5	46
64	Structures, phase stabilities, and electrical potentials of Li-Si battery anode materials. <i>Physical Review B</i> , 2013, 87, .	1.1	41
65	Computational Discovery, Characterization, and Design of Single-Layer Materials. <i>Jom</i> , 2014, 66, 366-374.	0.9	41
66	Controllable p-Type Doping of 2D WSe ₂ via Vanadium Substitution. <i>Advanced Functional Materials</i> , 2021, 31, 2105252.	7.8	40
67	Hydrogen storage in Ti-Zr and Ti-Hf-based quasicrystals. <i>Philosophical Magazine</i> , 2006, 86, 957-964.	0.7	39
68	Functional form of the superconducting critical temperature from machine learning. <i>Physical Review B</i> , 2019, 100, .	1.1	35
69	Accuracy of quantum Monte Carlo methods for point defects in solids. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 267-274.	0.7	34
70	Ab initio prediction of environmental embrittlement at a crack tip in aluminum. <i>Physical Review B</i> , 2012, 86, .	1.1	34
71	Predicting the Electrochemical Synthesis of 2D Materials from First Principles. <i>Journal of Physical Chemistry C</i> , 2019, 123, 3180-3187.	1.5	34
72	Pressure-induced structural transitions in europium to 92 GPa. <i>Physical Review B</i> , 2011, 83, .	1.1	33

#	ARTICLE	IF	CITATIONS
73	(NH ₄) ₂ S, a highly reactive molecular precursor for low temperature anion exchange reactions in nanoparticles. Dalton Transactions, 2013, 42, 12596.	1.6	33
74	Increased activity in hydrogen evolution electrocatalysis for partial anionic substitution in cobalt oxysulfide nanoparticles. Journal of Materials Chemistry A, 2016, 4, 2842-2848.	5.2	32
75	Scalable Substitutional Re ⁺ Doping and its Impact on the Optical and Electronic Properties of Tungsten Diselenide. Advanced Materials, 2020, 32, e2005159.	11.1	32
76	Energy landscape of silicon systems and its description by force fields, tight binding schemes, density functional methods, and quantum Monte Carlo methods. Physical Review B, 2010, 81, .	1.1	31
77	Structure and Stability Prediction of Compounds with Evolutionary Algorithms. Topics in Current Chemistry, 2014, 345, 181-222.	4.0	31
78	Empirical tight-binding model for titanium phase transformations. Physical Review B, 2006, 73, .	1.1	30
79	Al ₂ O ₃ as a suitable substrate and a dielectric layer for n-layer MoS ₂ . Applied Physics Letters, 2015, 107, 053106.	1.5	30
80	Ab initio Ti-Zr-Ni phase diagram predicts stability of icosahedral TiZrNi quasicrystals. Physical Review B, 2005, 71, .	1.1	29
81	Systematic pathway generation and sorting in martensitic transformations: Titanium [±] to [±] %. Physical Review B, 2005, 72, .	1.1	27
82	Machine learning of superconducting critical temperature from Eliashberg theory. Npj Computational Materials, 2022, 8, .	3.5	27
83	Mesoscopic structure prediction of nanoparticle assembly and coassembly: Theoretical foundation. Journal of Chemical Physics, 2010, 133, 194108.	1.2	26
84	Spectroscopic Characterization of Charged Defects in Polycrystalline Pentacene by Time ⁺ and Wavelength ⁺ Resolved Electric Force Microscopy. Advanced Materials, 2011, 23, 624-628.	11.1	26
85	Scaling relation for thermal ripples in single and multilayer graphene. Physical Review B, 2013, 87, .	1.1	25
86	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 12530-12538.	1.5	25
87	Quantum Monte Carlo algorithms for electronic structure at the petascale; the Endstation project. Journal of Physics: Conference Series, 2008, 125, 012057.	0.3	24
88	Predicting Chiral Nanostructures, Lattices and Superlattices in Complex Multicomponent Nanoparticle Self-Assembly. Nano Letters, 2012, 12, 3218-3223.	4.5	24
89	Exploring Periodic Bicontinuous Cubic Network Structures with Complete Phononic Bandgaps. Journal of Physical Chemistry C, 2017, 121, 22347-22352.	1.5	24
90	Stability of charged sulfur vacancies in 2D and bulk MoS_2 from plane-wave density functional theory with electrostatic corrections. Physical Review Materials, 2020, 4, .	0.9	24

#	ARTICLE	IF	CITATIONS
91	Towards organic energy storage: characterization of 2,5-bis(methylthio)thieno[3,2-b]thiophene. <i>Journal of Materials Chemistry</i> , 2011, 21, 9553.	6.7	23
92	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. <i>Computational Materials Science</i> , 2016, 113, 80-87.	1.4	23
93	Genetic algorithm prediction of two-dimensional group-IV dioxides for dielectrics. <i>Physical Review B</i> , 2017, 95, .	1.1	23
94	Theoretical and Electrochemical Analysis of Poly(3,4-alkylenedioxythiophenes): Electron-Donating Effects and Onset of p-Doped Conductivity. <i>Journal of Physical Chemistry C</i> , 2010, 114, 16776-16784.	1.5	21
95	Coupled quantum-continuum analysis of crack tip processes in aluminum. <i>Journal of the Mechanics and Physics of Solids</i> , 2011, 59, 2476-2487.	2.3	20
96	Synchrotron x-ray spectroscopy studies of valence and magnetic state in europium metal to extreme pressures. <i>Physical Review B</i> , 2012, 85, .	1.1	20
97	Density-matrix functional method for electronic properties of impurities. <i>Physical Review B</i> , 2001, 63, .	1.1	19
98	Machine learning of octahedral tilting in oxide perovskites by symbolic classification with compressed sensing. <i>Computational Materials Science</i> , 2020, 180, 109690.	1.4	19
99	Evaluation and comparison of classical interatomic potentials through a user-friendly interactive web-interface. <i>Scientific Data</i> , 2017, 4, 160125.	2.4	18
100	Silver delafossite nitride, AgTaN ₂ ?. <i>Journal of Solid State Chemistry</i> , 2011, 184, 7-11.	1.4	17
101	New experimental studies on the phase diagram of the Al-Cu-Fe quasicrystal-forming system. <i>Materials and Design</i> , 2020, 185, 108186.	3.3	17
102	First-principles study on the stabilization of approximants to icosahedral titanium-3d-transition-metal quasicrystals by silicon and oxygen. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 1997, 76, 1053-1064.	0.8	16
103	Theoretical and experimental investigation of the electronic structure of Ti-Zr-Ni and Ti-Zr-Ni:H alloys. <i>Journal of Alloys and Compounds</i> , 2002, 342, 337-342.	2.8	16
104	High Throughput Thin Film Pt-M Alloys for Fuel Electrooxidation: Low Concentrations of M (M = Sn, Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 159, F880-F887.	1.3	16
105	Structural Changes in 2D BiSe Bilayers as n Increases in (BiSe) _{1+δ} (NbSe) ₂ ($n = 4$) Heterostructures. <i>ACS Nano</i> , 2016, 10, 9489-9499.	7.3	16
106	Nanocrystal Symmetry Breaking and Accelerated Solid-State Diffusion in the Lead-Cadmium Sulfide Cation Exchange system. <i>Chemistry of Materials</i> , 2019, 31, 991-1005.	3.2	16
107	From compact point defects to extended structures in silicon. <i>European Physical Journal B</i> , 2007, 57, 229-234.	0.6	15
108	Energy landscape of silicon tetrahedral interstitials using an optimized classical potential. <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, 2050-2055.	0.7	14

#	ARTICLE	IF	CITATIONS
109	Framework for solvation in quantum Monte Carlo. <i>Physical Review B</i> , 2012, 85, .	1.1	14
110	<i>Ab initio</i> studies of Cs on GaAs (100) and (110) surfaces. <i>Physical Review B</i> , 2015, 91, .	1.1	14
111	Machine learning of ab-initio energy landscapes for crystal structure predictions. <i>Computational Materials Science</i> , 2019, 158, 414-419.	1.4	14
112	Augmenting machine learning of energy landscapes with local structural information. <i>Journal of Applied Physics</i> , 2020, 128, .	1.1	13
113	Computationally driven experimental discovery of the CeIr In_4 compound. <i>Physical Review B</i> , 2011, 83, .	1.1	12
114	Nanoparticle Metamorphosis: An <i>in Situ</i> High-Temperature Transmission Electron Microscopy Study of the Structural Evolution of Heterogeneous Au:Fe ₂ O ₃ Nanoparticles. <i>ACS Nano</i> , 2014, 8, 5315-5322.	7.3	12
115	Insights into the Charge-Transfer Stabilization of Heterostructure Components with Unstable Bulk Analogs. <i>Chemistry of Materials</i> , 2018, 30, 4738-4747.	3.2	12
116	Experimental investigation of the Al-Co-Fe phase diagram over the whole composition range. <i>Journal of Alloys and Compounds</i> , 2020, 815, 152110.	2.8	12
117	Controlling neutral and charged excitons in MoS ₂ with defects. <i>Journal of Materials Research</i> , 2020, 35, 949-957.	1.2	12
118	Fast diffusion mechanism of silicon tri-interstitial defects. <i>Physical Review B</i> , 2005, 72, .	1.1	11
119	Pressure-induced superconductivity in the giant Rashba system BiTeI. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 09LT02.	0.7	11
120	The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO ₂ . <i>Applied Sciences (Switzerland)</i> , 2019, 9, 5276.	1.3	11
121	Electronic structure of dangling bonds in amorphous silicon studied via a density-matrix functional method. <i>Physical Review B</i> , 2002, 66, .	1.1	10
122	Following Chemical Charge Trapping in Pentacene Thin Films by Selective Impurity Doping and Wavelength-Resolved Electric Force Microscopy. <i>Advanced Functional Materials</i> , 2012, 22, 5096-5106.	7.8	10
123	Computational discovery of lanthanide doped and Co-doped Y ₃ Al ₅ O ₁₂ for optoelectronic applications. <i>Applied Physics Letters</i> , 2015, 107, 112109.	1.5	10
124	Rietveld refinement and ab initio calculations of a C14-like Laves phase in Ti-Zr-Ni. <i>Philosophical Magazine Letters</i> , 2003, 83, 65-71.	0.5	9
125	Diffusion mechanisms for silicon di-interstitials. <i>Physical Review B</i> , 2006, 73, .	1.1	9
126	The Nanocrystal Superlattice Pressure Cell: A Novel Approach To Study Molecular Bundles under Uniaxial Compression. <i>Nano Letters</i> , 2014, 14, 4763-4766.	4.5	9

#	ARTICLE	IF	CITATIONS
127	First-principles investigation of charged dopants and dopant-vacancy defect complexes in monolayer MoS_2 . <i>Physical Review Materials</i> , 2020, 4, .		9
128	Barriers to predictive high-throughput screening for spin-crossover. <i>Computational Materials Science</i> , 2022, 206, 111161.	1.4	9
129	Ab initio prediction of the Li_5Ge_2 Zintl compound. <i>Computational Materials Science</i> , 2014, 93, 133-136.	1.4	8
130	Importance of high-angular-momentum channels in pseudopotentials for quantum Monte Carlo. <i>Physical Review B</i> , 2014, 90, .	1.1	8
131	Interface-Driven Structural Distortions and Composition Segregation in Two-Dimensional Heterostructures. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 14448-14452.	7.2	8
132	Strain modulation using defects in two-dimensional MoS_2 . <i>Physical Review B</i> , 2020, 102, .	1.1	8
133	Location and energy of interstitial hydrogen in the $1\hat{1}\hat{1}$ -approximant W-TiZrNi of the icosahedral TiZrNi quasicrystal: Rietveld refinement of x-ray and neutron diffraction data and density-functional calculations. <i>Physical Review B</i> , 2006, 73, .	1.1	7
134	Candidate replacements for lead in $\text{CH}_3\text{NH}_3\text{PbI}_3$ from first principles calculations. <i>Computational Materials Science</i> , 2018, 155, 69-73.	1.4	7
135	Multi-objective optimization of interatomic potentials with application to MgO. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019, 27, 074007.	0.8	7
136	Phase equilibria and diffusion coefficients in the Fe-Zn binary system. <i>Materials and Design</i> , 2020, 188, 108437.	3.3	7
137	Photoluminescence Induced by Substitutional Nitrogen in Single-Layer Tungsten Disulfide. <i>ACS Nano</i> , 2022, 16, 7428-7437.	7.3	7
138	Role of composition and structure on the properties of metal/multifunctional ceramic interfaces. <i>Journal of Applied Physics</i> , 2016, 120, .	1.1	6
139	Limitations of empirical supercell extrapolation for calculations of point defects in bulk, at surfaces, and in two-dimensional materials. <i>Physical Review B</i> , 2022, 105, .	1.1	6
140	Phase Behavior of Pseudobinary Precious Metal Carbide Systems. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21664-21671.	1.5	5
141	Role of magnetism on transition metal oxide surfaces in vacuum and solvent. <i>Physical Review Materials</i> , 2020, 4, .	0.9	5
142	Charged vacancy defects in monolayer phosphorene. <i>Physical Review Materials</i> , 2021, 5, .	0.9	5
143	Physically and chemically smooth cesium-antimonide photocathodes on single crystal strontium titanate substrates. <i>Applied Physics Letters</i> , 2022, 120, .	1.5	5
144	First-principles study of superconductivity in In_2Ga and In_2Ga gallium. <i>Physical Review B</i> , 2021, 104, .	1.1	4

#	ARTICLE	IF	CITATIONS
145	High-throughput density functional calculations to optimize properties and interfacial chemistry of piezoelectric materials. <i>Physical Review Materials</i> , 2018, 2, .	0.9	4
146	High throughput screening of substrates for synthesis and functionalization of 2D materials. <i>Proceedings of SPIE</i> , 2015, , .	0.8	3
147	Comparison of polynomial approximations to speed up planewave-based quantum Monte Carlo calculations. <i>Journal of Computational Physics</i> , 2015, 287, 77-87.	1.9	2
148	High-pressure study of the low- Z rich superconductor Be ₂₂ Re. <i>Physical Review B</i> , 2021, 104, .	1.1	2
149	Computational synthesis of substrates by crystal cleavage. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	2
150	Ligand Optimization of Exchange Interaction in Co(II) Dimer Single Molecule Magnet by Machine Learning. <i>Journal of Physical Chemistry A</i> , 2022, 126, 529-535.	1.1	2
151	Giant Stokes shift for charged vacancies in monolayer SnS. <i>Physical Review Materials</i> , 2022, 6, .	0.9	2
152	Interface-Driven Structural Distortions and Composition Segregation in Two-Dimensional Heterostructures. <i>Angewandte Chemie</i> , 2017, 129, 14640-14644.	1.6	1
153	Remarkable low-energy properties of the pseudogapped semimetal Be ₅ Pt. <i>Physical Review B</i> , 2020, 102, .	1.1	1
154	Split-vacancy defect complexes of oxygen in hcp and fcc cobalt. <i>Physical Review Materials</i> , 2020, 4, .	0.9	1
155	Fundamental Cluster and Hydrogen Sites in Ti-Zr-Ni Quasicrystals. <i>Materials Research Society Symposia Proceedings</i> , 2000, 643, 521.	0.1	0
156	Large-Scale Molecular Dynamics Simulations of Interstitial Defect Diffusion in Silicon. <i>Materials Research Society Symposia Proceedings</i> , 2002, 731, 9101.	0.1	0
157	Applying for computational time on NSF's TeraGrid—the world's largest cyberinfrastructure supporting open research. <i>Jom</i> , 2010, 62, 17-18.	0.9	0
158	Back Cover: Accuracy of quantum Monte Carlo methods for point defects in solids (Phys. Status Tj ETQq0 0 0 rgBT/Overlock 10 Tf 50 2	0.7	0
159	A ₁₅ Nb ₃ Si: a high T _c superconductor synthesized at a pressure of one megabar and metastable at ambient conditions. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 285705.	0.7	0
160	Ab-initio Study of the Ground-State Phase Diagram of the Icosahedral Ti-Zr-Ni Quasicrystal. <i>Springer Proceedings in Physics</i> , 2002, , 204-208.	0.1	0