Richard G Hennig

List of Publications by Year
in descending order

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160 papers	14,027 citations	25034 57 h-index	20358 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.	3.0	1,676
2	Single-Layer Group-III Monochalcogenide Photocatalysts for Water Splitting. Chemistry of Materials, 2013, 25, 3232-3238.	6.7	675
3	Computational Screening of 2D Materials for Photocatalysis. Journal of Physical Chemistry Letters, 2015, 6, 1087-1098.	4.6	641
4	Implicit self-consistent electrolyte model in plane-wave density-functional theory. Journal of Chemical Physics, 2019, 151, 234101.	3.0	561
5	Computational Search for Single-Layer Transition-Metal Dichalcogenide Photocatalysts. Journal of Physical Chemistry C, 2013, 117, 20440-20445.	3.1	468
6	Ab Initio Prediction of Piezoelectricity in Two-Dimensional Materials. ACS Nano, 2015, 9, 9885-9891.	14.6	445
7	Alleviation of the Fermion-Sign Problem by Optimization of Many-Body Wave Functions. Physical Review Letters, 2007, 98, 110201.	7.8	411
8	Computational discovery of single-layer III-V materials. Physical Review B, 2013, 87, .	3.2	318
9	Softened Elastic Response and Unzipping in Chemical Vapor Deposition Graphene Membranes. Nano Letters, 2011, 11, 2259-2263.	9.1	316
10	Angle-Resolved Raman Imaging of Interlayer Rotations and Interactions in Twisted Bilayer Graphene. Nano Letters, 2012, 12, 3162-3167.	9.1	299
11	Strong anisotropy and magnetostriction in the two-dimensional Stoner ferromagnet<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>GeTe₂. Physical Review B, 2016, 93, .	3.2	299
12	Enhanced Liâ€“S Batteries Using Amine-Functionalized Carbon Nanotubes in the Cathode. ACS Nano, 2016, 10, 1050-1059.	14.6	289
13	Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials. Physical Review Letters, 2017, 118, 106101.	7.8	262
14	Computational prediction of two-dimensional group-IV mono-chalcogenides. Applied Physics Letters, 2014, 105, .	3.3	245
15	Predicting Nanocrystal Shape through Consideration of Surface-Ligand Interactions. ACS Nano, 2012, 6, 2118-2127.	14.6	236
16	Theoretical perspective of photocatalytic properties of single-layer SnS<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, .	3.2	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.	14.6	211
18	Accuracy of exchange-correlation functionals and effect of solvation on the surface energy of copper. Physical Review B, 2013, 87, .	3.2	211

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19	Impurities block the Î± to Ï‰ martensitic transformation in titanium. Nature Materials, 2005, 4, 129-133.	27.5	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.	13.7	198
21	Predicted Surface Composition and Thermodynamic Stability of MXenes in Solution. Journal of Physical Chemistry C, 2016, 120, 3550-3556.	3.1	196
22	Strong spin-lattice coupling in CrSiTe3. APL Materials, 2015, 3, .	5.1	192
23	Stability and magnetism of strongly correlated single-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>VS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2016, 93, .	3.2	176
24	Classical potential describes martensitic phase transformations between the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math>, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ï‰</mml:mi></mml:math>titanium phases. Physical Review B, 2008, 78, .	3.2	173
25	Two-Dimensional Intrinsic Half-Metals With Large Spin Gaps. Nano Letters, 2017, 17, 5251-5257.	9.1	172
26	New Mechanism for theÎ±toÏ‰Martensitic Transformation in Pure Titanium. Physical Review Letters, 2003, 91, 025701.	7.8	156
27	Solidâ€“Solid Phase Transformations Induced through Cation Exchange and Strain in 2D Heterostructured Copper Sulfide Nanocrystals. Nano Letters, 2014, 14, 7090-7099.	9.1	147
28	ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials. Physical Chemistry Chemical Physics, 2015, 17, 3383-3393.	2.8	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, .	3.2	131
31	Synthesis of borophane polymorphs through hydrogenation of borophene. Science, 2021, 371, 1143-1148.	12.6	129
32	The Oxidation of Cobalt Nanoparticles into Kirkendall-Hollowed CoO and Co₃O₄: The Diffusion Mechanisms and Atomic Structural Transformations. Journal of Physical Chemistry C, 2013, 117, 14303-14312.	3.1	128
33	Hybrid cathode architectures for lithium batteries based on TiS₂ and sulfur. Journal of Materials Chemistry A, 2015, 3, 19857-19866.	10.3	119
34	Threeâ€Dimensionally Isotropic Negative Refractive Index Materials from Block Copolymer Selfâ€Assembled Chiral Gyroid Networks. Angewandte Chemie - International Edition, 2011, 50, 11985-11989.	13.8	116
35	Electronic structures of single-layer boron pnictides. Applied Physics Letters, 2012, 101, .	3.3	114
36	Ab initiosynthesis of single-layer III-V materials. Physical Review B, 2014, 89, .	3.2	112

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37	Emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys. Nature, 2008, 451, 445-448.	27.8	111
38	Computational prediction and characterization of single-layer CrS₂. Applied Physics Letters, 2014, 104, 022116.	3.3	108
39	Density functional theory study of the electrochemical interface between a Pt electrode and an aqueous electrolyte using an implicit solvent method. Journal of Chemical Physics, 2015, 142, 234107.	3.0	103
40	MPInterfaces: A Materials Project based Python tool for high-throughput computational screening of interfacial systems. Computational Materials Science, 2016, 122, 183-190.	3.0	95
41	Computational Study of Low Interlayer Friction in Ti_{n+1}C_n (n = 1, 2, and 3) MXene. ACS Applied Materials & Interfaces, 2017, 9, 34467-34479.	8.0	93
42	Theoretical Studies of Carbonyl-Based Organic Molecules for Energy Storage Applications: The Heteroatom and Substituent Effect. Journal of Physical Chemistry C, 2014, 118, 6046-6051.	3.1	91
43	Dynamic instabilities in strongly correlated <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>VSe</mml:mtext><mml:mn>2</mml:mn></mml:ms monolayers and bilayers. Physical Review B, 2017, 96, .	3.2	91
44	Unintended Phosphorus Doping of Nickel Nanoparticles during Synthesis with TOP: A Discovery through Structural Analysis. Nano Letters, 2012, 12, 4530-4539.	9.1	81
45	Computational characterization of lightweight multilayer MXene Li-ion battery anodes. Applied Physics Letters, 2016, 108, .	3.3	79
46	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	1.8	79
47	Li-Carboxylate Anode Structure-Property Relationships from Molecular Modeling. Chemistry of Materials, 2013, 25, 132-141.	6.7	75
48	Computational discovery of stable<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>M</mml:mi><mml:mn>2</mml:mn></mml:ms Physical Review B, 2016, 94, .	3.2	75
49	Ab initiobased empirical potential used to study the mechanical properties of molybdenum. Physical Review B, 2012, 85, .	3.2	71
50	Complexity of Small Silicon Self-Interstitial Defects. Physical Review Letters, 2004, 92, 045501.	7.8	69
51	Tethered Molecular Sorbents: Enabling Metalâ€Sulfur Battery Cathodes. Advanced Energy Materials, 2014, 4, 1400390.	19.5	67
52	Phase transformation in Si from semiconducting diamond to metallic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î²</mml:mi><mml:mtext>-Sn</mml:mtext></mml:mrow></mml:math>phase in QMC and DFT under hydrostatic and anisotropic stress. Physical Review B, 2010, 82, .	3.2	65
53	Questioning the existence of a unique ground-state structure for Si clusters. Physical Review B, 2007, 75, .	3.2	62
54	Doping-controlled phase transitions in single-layer <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></mm Physical Review B, 2017, 96, .	3.2	62

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55	Rashba effect in single-layer antimony telluroiodide SbTeI. Physical Review B, 2015, 92, .	3.2	60
56	Computational discovery and characterization of polymorphic two-dimensional IVâ€“V materials. Applied Physics Letters, 2016, 109, .	3.3	60
57	Grand-canonical evolutionary algorithm for the prediction of two-dimensional materials. Physical Review B, 2016, 93, .	3.2	59
58	Tailored redox functionality of small organics for pseudocapacitive electrodes. Energy and Environmental Science, 2012, 5, 7176.	30.8	58
59	Computational methods for 2D materials: discovery, property characterization, and application design. Journal of Physics Condensed Matter, 2017, 29, 473001.	1.8	55
60	Computational identification of single-layer CdO for electronic and optical applications. Applied Physics Letters, 2013, 103, .	3.3	52
61	A grand canonical genetic algorithm for the prediction of multi-component phase diagrams and testing of empirical potentials. Journal of Physics Condensed Matter, 2013, 25, 495401.	1.8	52
62	Structure of the icosahedral Ti-Zr-Ni quasicrystal. Physical Review B, 2003, 67, .	3.2	46
63	Computational synthesis of single-layer GaN on refractory materials. Applied Physics Letters, 2014, 105, .	3.3	46
64	Structures, phase stabilities, and electrical potentials of Li-Si battery anode materials. Physical Review B, 2013, 87, .	3.2	41
65	Computational Discovery, Characterization, and Design of Single-Layer Materials. Jom, 2014, 66, 366-374.	1.9	41
66	Controllable pâ€Type Doping of 2D WSe₂ via Vanadium Substitution. Advanced Functional Materials, 2021, 31, 2105252.	14.9	40
67	Hydrogen storage in Tiâ€“Zr and Tiâ€“Hf-based quasicrystals. Philosophical Magazine, 2006, 86, 957-964.	1.6	39
68	Functional form of the superconducting critical temperature from machine learning. Physical Review B, 2019, 100, .	3.2	35
69	Accuracy of quantum Monte Carlo methods for point defects in solids. Physica Status Solidi (B): Basic Research, 2011, 248, 267-274.	1.5	34
70	Ab initioprediction of environmental embrittlement at a crack tip in aluminum. Physical Review B, 2012, 86, .	3.2	34
71	Predicting the Electrochemical Synthesis of 2D Materials from First Principles. Journal of Physical Chemistry C, 2019, 123, 3180-3187.	3.1	34
72	Pressure-induced structural transitions in europium to 92 GPa. Physical Review B, 2011, 83, .	3.2	33

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73	(NH4)2S, a highly reactive molecular precursor for low temperature anion exchange reactions in nanoparticles. Dalton Transactions, 2013, 42, 12596.	3.3	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.	10.3	32
75	Scalable Substitutional Reâ€Doping and its Impact on the Optical and Electronic Properties of Tungsten Diselenide. Advanced Materials, 2020, 32, e2005159.	21.0	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, .	3.2	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, .	3.2	30
79	Al2O3 as a suitable substrate and a dielectric layer for n-layer MoS2. Applied Physics Letters, 2015, 107, 053106.	3.3	30
80	Ab initioTi-Zr-Ni phase diagram predicts stability of icosahedral TiZrNi quasicrystals. Physical Review B, 2005, 71, .	3.2	29
81	Systematic pathway generation and sorting in martensitic transformations: TitaniumÎ±toï‰. Physical Review B, 2005, 72, .	3.2	27
82	Machine learning of superconducting critical temperature from Eliashberg theory. Npj Computational Materials, 2022, 8, .	8.7	27
83	Mesoscopic structure prediction of nanoparticle assembly and coassembly: Theoretical foundation. Journal of Chemical Physics, 2010, 133, 194108.	3.0	26
84	Spectroscopic Characterization of Charged Defects in Polycrystalline Pentacene by Timeâ€and Wavelengthâ€Resolved Electric Force Microscopy. Advanced Materials, 2011, 23, 624-628.	21.0	26
85	Scaling relation for thermal ripples in single and multilayer graphene. Physical Review B, 2013, 87, .	3.2	25
86	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 12530-12538.	3.1	25
87	Quantum Monte Carlo algorithms for electronic structure at the petascale; the Endstation project. Journal of Physics: Conference Series, 2008, 125, 012057.	0.4	24
88	Predicting Chiral Nanostructures, Lattices and Superlattices in Complex Multicomponent Nanoparticle Self-Assembly. Nano Letters, 2012, 12, 3218-3223.	9.1	24
89	Exploring Periodic Bicontinuous Cubic Network Structures with Complete Phononic Bandgaps. Journal of Physical Chemistry C, 2017, 121, 22347-22352.	3.1	24
90	Stability of charged sulfur vacancies in 2D and bulk <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></mm from plane-wave density functional theory with electrostatic corrections. Physical Review Materials, 2020, 4, .	2.4	24

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91	Towards organic energy storage: characterization of 2,5-bis(methylthio)thieno[3,2-b]thiophene. Journal of Materials Chemistry, 2011, 21, 9553.	6.7	23
92	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. Computational Materials Science, 2016, 113, 80-87.	3.0	23
93	Genetic algorithm prediction of two-dimensional group-IV dioxides for dielectrics. Physical Review B, 2017, 95, .	3.2	23
94	Theoretical and Electrochemical Analysis of Poly(3,4-alkylenedioxythiophenes): Electron-Donating Effects and Onset of p-Doped Conductivity. Journal of Physical Chemistry C, 2010, 114, 16776-16784.	3.1	21
95	Coupled quantumâ€“continuum analysis of crack tip processes in aluminum. Journal of the Mechanics and Physics of Solids, 2011, 59, 2476-2487.	4.8	20
96	Synchrotron x-ray spectroscopy studies of valence and magnetic state in europium metal to extreme pressures. Physical Review B, 2012, 85, .	3.2	20
97	Density-matrix functional method for electronic properties of impurities. Physical Review B, 2001, 63, .	3.2	19
98	Machine learning of octahedral tilting in oxide perovskites by symbolic classification with compressed sensing. Computational Materials Science, 2020, 180, 109690.	3.0	19
99	Evaluation and comparison of classical interatomic potentials through a user-friendly interactive web-interface. Scientific Data, 2017, 4, 160125.	5.3	18
100	Silver delafossite nitride, AgTaN2?. Journal of Solid State Chemistry, 2011, 184, 7-11.	2.9	17
101	New experimental studies on the phase diagram of the Al-Cu-Fe quasicrystal-forming system. Materials and Design, 2020, 185, 108186.	7.0	17
102	First-principles study on the stabilization of approximants to icosahedral titaniumâ€”3d-transition-metal quasicrystals by silicon and oxygen. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1997, 76, 1053-1064.	0.6	16
103	Theoretical and experimental investigation of the electronic structure of Tiâ€“Zrâ€“Ni and Tiâ€“Zrâ€“Ni:H alloys. Journal of Alloys and Compounds, 2002, 342, 337-342.	5.5	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.	2.9	16
105	Structural Changes in 2D BiSe Bilayers as n Increases in (BiSe)_{1+Î´}(NbSe₂)_n (n = 1â€“4) Heterostructures. ACS Nano, 2016, 10, 9489-9499.	14.6	16
106	Nanocrystal Symmetry Breaking and Accelerated Solid-State Diffusion in the Leadâ€“Cadmium Sulfide Cation Exchange system. Chemistry of Materials, 2019, 31, 991-1005.	6.7	16
107	From compact point defects to extended structures in silicon. European Physical Journal B, 2007, 57, 229-234.	1.5	15
108	Energy landscape of silicon tetraâ€interstitials using an optimized classical potential. Physica Status Solidi (B): Basic Research, 2011, 248, 2050-2055.	1.5	14

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109	Framework for solvation in quantum Monte Carlo. Physical Review B, 2012, 85, .	3.2	14
110	Ab initiostudies of Cs on GaAs (100) and (110) surfaces. Physical Review B, 2015, 91, .	3.2	14
111	Machine learning of ab-initio energy landscapes for crystal structure predictions. Computational Materials Science, 2019, 158, 414-419.	3.0	14
112	Augmenting machine learning of energy landscapes with local structural information. Journal of Applied Physics, 2020, 128, .	2.5	13
113	Computationally driven experimental discovery of the CeIr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>In compound. Physical Review B, 2011, 83, .	3.2	12
114	Nanoparticle Metamorphosis: An in Situ High-Temperature Transmission Electron Microscopy Study of the Structural Evolution of Heterogeneous Au:Fe₂O₃ Nanoparticles. ACS Nano, 2014, 8, 5315-5322.	14.6	12
115	Insights into the Charge-Transfer Stabilization of Heterostructure Components with Unstable Bulk Analogs. Chemistry of Materials, 2018, 30, 4738-4747.	6.7	12
116	Experimental investigation of the Alâ€“Coâ€“Fe phase diagram over the whole composition range. Journal of Alloys and Compounds, 2020, 815, 152110.	5.5	12
117	Controlling neutral and charged excitons in MoS₂ with defects. Journal of Materials Research, 2020, 35, 949-957.	2.6	12
118	Fast diffusion mechanism of silicon tri-interstitial defects. Physical Review B, 2005, 72, .	3.2	11
119	Pressure-induced superconductivity in the giant Rashba system BiTeI. Journal of Physics Condensed Matter, 2017, 29, 09LT02.	1.8	11
120	The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO2. Applied Sciences (Switzerland), 2019, 9, 5276.	2.5	11
121	Electronic structure of dangling bonds in amorphous silicon studied via a density-matrix functional method. Physical Review B, 2002, 66, .	3.2	10
122	Following Chemical Charge Trapping in Pentacene Thin Films by Selective Impurity Doping and Wavelengthâ€Resolved Electric Force Microscopy. Advanced Functional Materials, 2012, 22, 5096-5106.	14.9	10
123	Computational discovery of lanthanide doped and Co-doped Y3Al5O12 for optoelectronic applications. Applied Physics Letters, 2015, 107, 112109.	3.3	10
124	Rietveld refinement and ab initio calculations of a C14-like Laves phase in Ti-Zr-Ni. Philosophical Magazine Letters, 2003, 83, 65-71.	1.2	9
125	Diffusion mechanisms for silicon di-interstitials. Physical Review B, 2006, 73, .	3.2	9
126	The Nanocrystal Superlattice Pressure Cell: A Novel Approach To Study Molecular Bundles under Uniaxial Compression. Nano Letters, 2014, 14, 4763-4766.	9.1	9

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127	First-principles investigation of charged dopants and dopant-vacancy defect complexes in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2020, 4, .	2.4	9
128	Barriers to predictive high-throughput screening for spin-crossover. Computational Materials Science, 2022, 206, 111161.	3.0	9
129	Ab initio prediction of the Li5Ge2 Zintl compound. Computational Materials Science, 2014, 93, 133-136.	3.0	8
130	Importance of high-angular-momentum channels in pseudopotentials for quantum Monte Carlo. Physical Review B, 2014, 90, .	3.2	8
131	Interfaceâ€Driven Structural Distortions and Composition Segregation in Twoâ€Dimensional Heterostructures. Angewandte Chemie - International Edition, 2017, 56, 14448-14452.	13.8	8
132	Strain modulation using defects in two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2020, 102, .	3.2	8
133	Location and energy of interstitial hydrogen in the1âˆ•1approximantW-TiZrNiof the icosahedralTiZrNiquasicrystal: Rietveld refinement of x-ray and neutron diffraction data and density-functional calculations. Physical Review B, 2006, 73, .	3.2	7
134	Candidate replacements for lead in CH3NH3PbI3 from first principles calculations. Computational Materials Science, 2018, 155, 69-73.	3.0	7
135	Multi-objective optimization of interatomic potentials with application to MgO. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 074007.	2.0	7
136	Phase equilibria and diffusion coefficients in the Fe-Zn binary system. Materials and Design, 2020, 188, 108437.	7.0	7
137	Photoluminescence Induced by Substitutional Nitrogen in Single-Layer Tungsten Disulfide. ACS Nano, 2022, 16, 7428-7437.	14.6	7
138	Role of composition and structure on the properties of metal/multifunctional ceramic interfaces. Journal of Applied Physics, 2016, 120, .	2.5	6
139	Limitations of empirical supercell extrapolation for calculations of point defects in bulk, at surfaces, and in two-dimensional materials. Physical Review B, 2022, 105, .	3.2	6
140	Phase Behavior of Pseudobinary Precious Metalâ“Carbide Systems. Journal of Physical Chemistry C, 2010, 114, 21664-21671.	3.1	5
141	Role of magnetism on transition metal oxide surfaces in vacuum and solvent. Physical Review Materials, 2020, 4, .	2.4	5
142	Charged vacancy defects in monolayer phosphorene. Physical Review Materials, 2021, 5, .	2.4	5
143	Physically and chemically smooth cesium-antimonide photocathodes on single crystal strontium titanate substrates. Applied Physics Letters, 2022, 120, .	3.3	5
144	First-principles study of superconductivity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math> gallium. Physical Review B, 2021, 104, .	3.2	4

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145	High-throughput density functional calculations to optimize properties and interfacial chemistry of piezoelectric materials. Physical Review Materials, 2018, 2, .	2.4	4
146	High throughput screening of substrates for synthesis and functionalization of 2D materials. Proceedings of SPIE, 2015, , .	0.8	3
147	Comparison of polynomial approximations to speed up planewave-based quantum Monte Carlo calculations. Journal of Computational Physics, 2015, 287, 77-87.	3.8	2
148	High-pressure study of the low- Z rich superconductor Be22Re. Physical Review B, 2021, 104, .	3.2	2
149	Computational synthesis of substrates by crystal cleavage. Npj Computational Materials, 2021, 7, .	8.7	2
150	Ligand Optimization of Exchange Interaction in Co(II) Dimer Single Molecule Magnet by Machine Learning. Journal of Physical Chemistry A, 2022, 126, 529-535.	2.5	2
151	Giant Stokes shift for charged vacancies in monolayer SnS. Physical Review Materials, 2022, 6, .	2.4	2
152	Interfaceâ€Driven Structural Distortions and Composition Segregation in Twoâ€Dimensional Heterostructures. Angewandte Chemie, 2017, 129, 14640-14644.	2.0	1
153	Remarkable low-energy properties of the pseudogapped semimetal Be5Pt. Physical Review B, 2020, 102, .	3.2	1
154	Split-vacancy defect complexes of oxygen in hcp and fcc cobalt. Physical Review Materials, 2020, 4, .	2.4	1
155	Fundamental Cluster and Hydrogen Sites in Ti-Zr-Ni Quasicrystals. Materials Research Society Symposia Proceedings, 2000, 643, 521.	0.1	0
156	Large-Scale Molecular Dynamics Simulations of Interstitial Defect Diffusion in Silicon. Materials Research Society Symposia Proceedings, 2002, 731, 9101.	0.1	0
157	Applying for computational time on NSFâ€™s TeraGridâ€”the worldâ€™s largest cyberinfrastructure supporting open research. Jom, 2010, 62, 17-18.	1.9	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	1.5	0
159	A15 Nb3Si: a â€˜highâ€™ T c superconductor synthesized at a pressure of one megabar and metastable at ambient conditions. Journal of Physics Condensed Matter, 2021, 33, 285705.	1.8	0
160	Ab-initio Study of the Ground-State Phase Diagram of the Icosahedral Ti-Zr-Ni Quasicrystal. Springer Proceedings in Physics, 2002, , 204-208.	0.2	0