Richard G Hennig

List of Publications by Citations

152 papers	10,279 citations	51 h-index	99 g-index
169 ext. papers	12,118 ext. citations	6.4 avg, IF	6.74 L-index

#	Paper	IF	Citations
152	Implicit solvation model for density-functional study of nanocrystal surfaces and reaction pathways. *Journal of Chemical Physics*, **2014**, 140, 084106	3.9	945
151	Single-Layer Group-III Monochalcogenide Photocatalysts for Water Splitting. *Chemistry of Materials*, **2013**, 25, 3232-3238	9.6	510
150	Computational Screening of 2D Materials for Photocatalysis. *Journal of Physical Chemistry Letters*, **2015**, 6, 1087-98	6.4	458
149	Computational Search for Single-Layer Transition-Metal Dichalcogenide Photocatalysts. *Journal of Physical Chemistry C*, **2013**, 117, 20440-20445	3.8	365
148	Alleviation of the Fermion-sign problem by optimization of many-body wave functions. *Physical Review Letters*, **2007**, 98, 110201	7.4	355
147	Ab Initio Prediction of Piezoelectricity in Two-Dimensional Materials. *ACS Nano*, **2015**, 9, 9885-91	16.7	297
146	Softened elastic response and unzipping in chemical vapor deposition graphene membranes. *Nano Letters*, **2011**, 11, 2259-63	11.5	278
145	Angle-resolved Raman imaging of interlayer rotations and interactions in twisted bilayer graphene. *Nano Letters*, **2012**, 12, 3162-7	11.5	260
144	Enhanced Li-S Batteries Using Amine-Functionalized Carbon Nanotubes in the Cathode. *ACS Nano*, **2016**, 10, 1050-9	16.7	251
143	Computational discovery of single-layer III-V materials. *Physical Review B*, **2013**, 87,	3.3	250
142	Implicit self-consistent electrolyte model in plane-wave density-functional theory. *Journal of Chemical Physics*, **2019**, 151, 234101	3.9	210
141	Predicting nanocrystal shape through consideration of surface-ligand interactions. *ACS Nano*, **2012**, 6, 2118-27	16.7	201
140	Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials. *Physical Review Letters*, **2017**, 118, 106101	7.4	193
139	Computational prediction of two-dimensional group-IV mono-chalcogenides. *Applied Physics Letters* , **2014**, 105, 042103	3.4	192
138	Strong anisotropy and magnetostriction in the two-dimensional Stoner ferromagnet Fe3GeTe2. *Physical Review B*, **2016**, 93,	3.3	183
137	van der Waals epitaxial growth of graphene on sapphire by chemical vapor deposition without a metal catalyst. *ACS Nano*, **2013**, 7, 385-95	16.7	182
136	Impurities block the alpha to omega martensitic transformation in titanium. *Nature Materials*, **2005**, 4, 129-33	27	179

135	Controlling nanocrystal superlattice symmetry and shape-anisotropic interactions through variable ligand surface coverage. *Journal of the American Chemical Society*, **2011**, 133, 3131-8	16.4	176
134	Theoretical perspective of photocatalytic properties of single-layer SnS2. *Physical Review B*, **2013**, 88,	3.3	173
133	Accuracy of exchange-correlation functionals and effect of solvation on the surface energy of copper. *Physical Review B*, **2013**, 87,	3.3	158
132	Predicted Surface Composition and Thermodynamic Stability of MXenes in Solution. *Journal of Physical Chemistry C*, **2016**, 120, 3550-3556	3.8	143
131	Strong spin-lattice coupling in CrSiTe3. *APL Materials*, **2015**, 3, 041515	5.7	142
130	Classical potential describes martensitic phase transformations between the □ and □ titanium phases. *Physical Review B*, **2008**, 78,	3.3	141
129	New mechanism for the alpha to omega martensitic transformation in pure titanium. *Physical Review Letters*, **2003**, 91, 025701	7.4	135
128	Solid-solid phase transformations induced through cation exchange and strain in 2D heterostructured copper sulfide nanocrystals. *Nano Letters*, **2014**, 14, 7090-9	11.5	122
127	The structural evolution and diffusion during the chemical transformation from cobalt to cobalt phosphide nanoparticles. *Journal of Materials Chemistry*, **2011**, 21, 11498		120
126	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,	3.3	119
125	Stability and magnetism of strongly correlated single-layer VS2. *Physical Review B*, **2016**, 93,	3.3	118
124	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	3.8	112
123	Hybrid cathode architectures for lithium batteries based on TiS2 and sulfur. *Journal of Materials Chemistry A*, **2015**, 3, 19857-19866	13	111
122	Two-Dimensional Intrinsic Half-Metals With Large Spin Gaps. *Nano Letters*, **2017**, 17, 5251-5257	11.5	111
121	ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials. *Physical Chemistry Chemical Physics*, **2015**, 17, 3383-93	3.6	109
120	Three-dimensionally isotropic negative refractive index materials from block copolymer self-assembled chiral gyroid networks. *Angewandte Chemie - International Edition*, **2011**, 50, 11985-9	16.4	99
119	Ab initio synthesis of single-layer III-V materials. *Physical Review B*, **2014**, 89,	3.3	98
118	Emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys. *Nature*, **2008**, 451, 445-8	50.4	93

117	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	3.9	92
116	Electronic structures of single-layer boron pnictides. *Applied Physics Letters*, **2012**, 101, 153109	3.4	92
115	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	3.8	81
114	Computational prediction and characterization of single-layer CrS2. *Applied Physics Letters*, **2014**, 104, 022116	3.4	80
113	MPInterfaces: A Materials Project based Python tool for high-throughput computational screening of interfacial systems. *Computational Materials Science*, **2016**, 122, 183-190	3.2	72
112	Unintended phosphorus doping of nickel nanoparticles during synthesis with TOP: a discovery through structural analysis. *Nano Letters*, **2012**, 12, 4530-9	11.5	69
111	Li-Carboxylate Anode Structure-Property Relationships from Molecular Modeling. *Chemistry of Materials*, **2013**, 25, 132-141	9.6	67
110	Tethered Molecular Sorbents: Enabling Metal-Sulfur Battery Cathodes. *Advanced Energy Materials*, **2014**, 4, 1400390	21.8	67
109	Computational characterization of lightweight multilayer MXene Li-ion battery anodes. *Applied Physics Letters*, **2016**, 108, 023901	3.4	66
108	Computational Study of Low Interlayer Friction in TiC (n = 1, 2, and 3) MXene. *ACS Applied Materials & Interfaces*, **2017**, 9, 34467-34479	9.5	62
107	Questioning the existence of a unique ground-state structure for Si clusters. *Physical Review B*, **2007**, 75,	3.3	62
106	Complexity of small silicon self-interstitial defects. *Physical Review Letters*, **2004**, 92, 045501	7.4	60
105	Phase transformation in Si from semiconducting diamond to metallic β-Sn phase in QMC and DFT under hydrostatic and anisotropic stress. *Physical Review B*, **2010**, 82,	3.3	58
104	Ab initio based empirical potential used to study the mechanical properties of molybdenum. *Physical Review B*, **2012**, 85,	3.3	57
103	Tailored redox functionality of small organics for pseudocapacitive electrodes. *Energy and Environmental Science*, **2012**, 5, 7176	35.4	52
102	Dynamic instabilities in strongly correlated VSe2 monolayers and bilayers. *Physical Review B*, **2017**, 96,	3.3	51
101	Computational discovery of stable M2AX phases. *Physical Review B*, **2016**, 94,	3.3	50
100	Doping-controlled phase transitions in single-layer MoS2. *Physical Review B*, **2017**, 96,	3.3	47

99	Grand-canonical evolutionary algorithm for the prediction of two-dimensional materials. *Physical Review B*, **2016**, 93,	3.3	47
98	Synthesis of borophane polymorphs through hydrogenation of borophene. *Science*, **2021**, 371, 1143-1148	33.3	46
97	Computational identification of single-layer CdO for electronic and optical applications. *Applied Physics Letters*, **2013**, 103, 212102	3.4	43
96	Computational synthesis of single-layer GaN on refractory materials. *Applied Physics Letters*, **2014**, 105, 051604	3.4	41
95	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	41
94	Structure of the icosahedral Ti-Zr-Ni quasicrystal. *Physical Review B*, **2003**, 67,	3.3	41
93	Computational discovery and characterization of polymorphic two-dimensional IVV materials. *Applied Physics Letters*, **2016**, 109, 192103	3.4	41
92	Computational methods for 2D materials: discovery, property characterization, and application design. *Journal of Physics Condensed Matter*, **2017**, 29, 473001	1.8	39
91	Hydrogen storage in TiZr and TiHf-based quasicrystals. *Philosophical Magazine*, **2006**, 86, 957-964	1.6	38
90	Computational Discovery, Characterization, and Design of Single-Layer Materials. *Jom*, **2014**, 66, 366-374	2.1	36
89	Structures, phase stabilities, and electrical potentials of Li-Si battery anode materials. *Physical Review B*, **2013**, 87,	3.3	34
88	(NH4)2S, a highly reactive molecular precursor for low temperature anion exchange reactions in nanoparticles. *Dalton Transactions*, **2013**, 42, 12596-9	4.3	32
87	Rashba effect in single-layer antimony telluroiodide SbTeI. *Physical Review B*, **2015**, 92,	3.3	31
86	Pressure-induced structural transitions in europium to 92 GPa. *Physical Review B*, **2011**, 83,	3.3	31
85	Ab initio prediction of environmental embrittlement at a crack tip in aluminum. *Physical Review B*, **2012**, 86,	3.3	29
84	Ab initio Ti-Zr-Ni phase diagram predicts stability of icosahedral TiZrNi quasicrystals. *Physical Review B*, **2005**, 71,	3.3	29
83	Accuracy of quantum Monte Carlo methods for point defects in solids. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 267-274	1.3	28
82	Empirical tight-binding model for titanium phase transformations. *Physical Review B*, **2006**, 73,	3.3	28

81	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,	3.3	27
80	Al2O3 as a suitable substrate and a dielectric layer for n-layer MoS2. *Applied Physics Letters*, **2015**, 107, 053106	3.4	26
79	Structure and stability prediction of compounds with evolutionary algorithms. *Topics in Current Chemistry*, **2014**, 345, 181-222		26
78	Mesoscopic structure prediction of nanoparticle assembly and coassembly: theoretical foundation. *Journal of Chemical Physics*, **2010**, 133, 194108	3.9	26
77	Spectroscopic characterization of charged defects in polycrystalline pentacene by time- and wavelength-resolved electric force microscopy. *Advanced Materials*, **2011**, 23, 624-8	24	25
76	Systematic pathway generation and sorting in martensitic transformations: Titanium □ to □ *Physical Review B*, **2005**, 72,	3.3	25
75	Increased activity in hydrogen evolution electrocatalysis for partial anionic substitution in cobalt oxysulfide nanoparticles. *Journal of Materials Chemistry A*, **2016**, 4, 2842-2848	13	24
74	Predicting chiral nanostructures, lattices and superlattices in complex multicomponent nanoparticle self-assembly. *Nano Letters*, **2012**, 12, 3218-23	11.5	23
73	Towards organic energy storage: characterization of 2,5-bis(methylthio)thieno[3,2-b]thiophene. *Journal of Materials Chemistry*, **2011**, 21, 9553		22
72	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 12530-12538	3.8	21
71	Scaling relation for thermal ripples in single and multilayer graphene. *Physical Review B*, **2013**, 87,	3.3	20
70	Coupled quantum□ontinuum analysis of crack tip processes in aluminum. *Journal of the Mechanics and Physics of Solids*, **2011**, 59, 2476-2487	5	20
69	Quantum Monte Carlo algorithms for electronic structure at the petascale; the Endstation project. *Journal of Physics: Conference Series*, **2008**, 125, 012057	0.3	20
68	Three-Dimensionally Isotropic Negative Refractive Index Materials from Block Copolymer Self-Assembled Chiral Gyroid Networks. *Angewandte Chemie*, **2011**, 123, 12191-12195	3.6	19
67	Exploring Periodic Bicontinuous Cubic Network Structures with Complete Phononic Bandgaps. *Journal of Physical Chemistry C*, **2017**, 121, 22347-22352	3.8	18
66	Density-matrix functional method for electronic properties of impurities. *Physical Review B*, **2001**, 63,	3.3	18
65	Predicting the Electrochemical Synthesis of 2D Materials from First Principles. *Journal of Physical Chemistry C*, **2019**, 123, 3180-3187	3.8	18
64	Genetic algorithm prediction of two-dimensional group-IV dioxides for dielectrics. *Physical Review B* , **2017**, 95,	3.3	17

63	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	3.8	17
62	Evaluation and comparison of classical interatomic potentials through a user-friendly interactive web-interface. *Scientific Data*, **2017**, 4, 160125	8.2	16
61	Silver delafossite nitride, AgTaN2?. *Journal of Solid State Chemistry*, **2011**, 184, 7-11	3.3	16
60	First-principles study on the stabilization of approximants to icosahedral titanium□d-transition-metal quasicrystals by silicon and oxygen. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1997**, 76, 1053-1064		16
59	Functional form of the superconducting critical temperature from machine learning. *Physical Review B*, **2019**, 100,	3.3	16
58	Theoretical and experimental investigation of the electronic structure of Ti□rNi and Ti□rNi:H alloys. *Journal of Alloys and Compounds*, **2002**, 342, 337-342	5.7	15
57	High Throughput Thin Film Pt-M Alloys for Fuel Electrooxidation: Low Concentrations of M (M = Sn, Ta, W, Mo, Ru, Fe, In, Pd, Hf, Zn, Zr, Nb, Sc, Ni, Ti, V, Cr, Rh). *Journal of the Electrochemical Society*, **2012**, 159, F880-F887	3.9	14
56	Synchrotron x-ray spectroscopy studies of valence and magnetic state in europium metal to extreme pressures. *Physical Review B*, **2012**, 85,	3.3	14
55	From compact point defects to extended structures in silicon. *European Physical Journal B*, **2007**, 57, 229-234	1.2	14
54	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. *Computational Materials Science*, **2016**, 113, 80-87	3.2	13
53	Framework for solvation in quantum Monte Carlo. *Physical Review B*, **2012**, 85,	3.3	13
52	Nanocrystal Symmetry Breaking and Accelerated Solid-State Diffusion in the Lead□admium Sulfide Cation Exchange system. *Chemistry of Materials*, **2019**, 31, 991-1005	9.6	12
51	Scalable Substitutional Re-Doping and its Impact on the Optical and Electronic Properties of Tungsten Diselenide. *Advanced Materials*, **2020**, 32, e2005159	24	11
50	Nanoparticle metamorphosis: an in situ high-temperature transmission electron microscopy study of the structural evolution of heterogeneous Au:Fe2O3 nanoparticles. *ACS Nano*, **2014**, 8, 5315-22	16.7	11
49	Computationally driven experimental discovery of the CeIr4In compound. *Physical Review B*, **2011**, 83,	3.3	11
48	Structural Changes in 2D BiSe Bilayers as n Increases in (BiSe)(NbSe) (n = 1-4) Heterostructures. *ACS Nano*, **2016**, 10, 9489-9499	16.7	11
47	New experimental studies on the phase diagram of the Al-Cu-Fe quasicrystal-forming system. *Materials and Design*, **2020**, 185, 108186	8.1	11
46	Pressure-induced superconductivity in the giant Rashba system BiTeI. *Journal of Physics Condensed Matter*, **2017**, 29, 09LT02	1.8	10

45	Ab initio studies of Cs on GaAs (100) and (110) surfaces. *Physical Review B*, **2015**, 91,	3.3	10
44	Machine learning of ab-initio energy landscapes for crystal structure predictions. *Computational Materials Science*, **2019**, 158, 414-419	3.2	10
43	Computational discovery of lanthanide doped and Co-doped Y3Al5O12 for optoelectronic applications. *Applied Physics Letters*, **2015**, 107, 112109	3.4	9
42	Following Chemical Charge Trapping in Pentacene Thin Films by Selective Impurity Doping and Wavelength-Resolved Electric Force Microscopy. *Advanced Functional Materials*, **2012**, 22, 5096-5106	15.6	9
41	Fast diffusion mechanism of silicon tri-interstitial defects. *Physical Review B*, **2005**, 72,	3.3	9
40	Electronic structure of dangling bonds in amorphous silicon studied via a density-matrix functional method. *Physical Review B*, **2002**, 66,	3.3	9
39	The 2021 Room-Temperature Superconductivity Roadmap. *Journal of Physics Condensed Matter*, **2021**,	1.8	9
38	Machine learning of octahedral tilting in oxide perovskites by symbolic classification with compressed sensing. *Computational Materials Science*, **2020**, 180, 109690	3.2	8
37	Interface-Driven Structural Distortions and Composition Segregation in Two-Dimensional Heterostructures. *Angewandte Chemie - International Edition*, **2017**, 56, 14448-14452	16.4	8
36	Rietveld refinement and ab initio calculations of a C14-like Laves phase in Ti-Zr-Ni. *Philosophical Magazine Letters*, **2003**, 83, 65-71	1	8
35	The nanocrystal superlattice pressure cell: a novel approach to study molecular bundles under uniaxial compression. *Nano Letters*, **2014**, 14, 4763-6	11.5	7
34	Importance of high-angular-momentum channels in pseudopotentials for quantum Monte Carlo. *Physical Review B*, **2014**, 90,	3.3	7
33	Diffusion mechanisms for silicon di-interstitials. *Physical Review B*, **2006**, 73,	3.3	7
32	The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO2. *Applied Sciences (Switzerland)*, **2019**, 9, 5276	2.6	7
31	Experimental investigation of the Al□Co□e phase diagram over the whole composition range. *Journal of Alloys and Compounds*, **2020**, 815, 152110	5.7	7
30	Insights into the Charge-Transfer Stabilization of Heterostructure Components with Unstable Bulk Analogs. *Chemistry of Materials*, **2018**, 30, 4738-4747	9.6	6
29	Ab initio prediction of the Li 5 Ge 2 Zintl compound. *Computational Materials Science*, **2014**, 93, 133-136	3.2	6
28	Role of composition and structure on the properties of metal/multifunctional ceramic interfaces. *Journal of Applied Physics*, **2016**, 120, 045310	2.5	6

27	Multi-objective optimization of interatomic potentials with application to MgO. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 074007	2	5
26	Controlling neutral and charged excitons in MoS2 with defects. *Journal of Materials Research*, **2020**, 35, 949-957	2.5	5
25	Candidate replacements for lead in CH3NH3PbI3 from first principles calculations. *Computational Materials Science*, **2018**, 155, 69-73	3.2	5
24	Energy landscape of silicon tetra-interstitials using an optimized classical potential. *Physica Status Solidi (B): Basic Research*, **2011**, 248, n/a-n/a	1.3	5
23	Location and energy of interstitial hydrogen in the 1□1 approximant W-TiZrNi of the icosahedral TiZrNi quasicrystal: Rietveld refinement of x-ray and neutron diffraction data and density-functional calculations. *Physical Review B*, **2006**, 73,	3.3	5
22	Augmenting machine learning of energy landscapes with local structural information. *Journal of Applied Physics*, **2020**, 128, 085101	2.5	5
21	Random Search Methods **2010**, 55-66		4
20	Controllable p-Type Doping of 2D WSe2 via Vanadium Substitution. *Advanced Functional Materials*, **2021**, 31, 2105252	15.6	4
19	Phase Behavior of Pseudobinary Precious Metal□arbide Systems. *Journal of Physical Chemistry C*, **2010**, 114, 21664-21671	3.8	3
18	Stability of charged sulfur vacancies in 2D and bulk MoS2 from plane-wave density functional theory with electrostatic corrections. *Physical Review Materials*, **2020**, 4,	3.2	3
17	Phase equilibria and diffusion coefficients in the Fe-Zn binary system. *Materials and Design*, **2020**, 188, 108437	8.1	3
16	Comparison of polynomial approximations to speed up planewave-based quantum Monte Carlo calculations. *Journal of Computational Physics*, **2015**, 287, 77-87	4.1	2
15	High throughput screening of substrates for synthesis and functionalization of 2D materials **2015**,		2
14	Role of magnetism on transition metal oxide surfaces in vacuum and solvent. *Physical Review Materials*, **2020**, 4,	3.2	2
13	Interface-Driven Structural Distortions and Composition Segregation in Two-Dimensional Heterostructures. *Angewandte Chemie*, **2017**, 129, 14640-14644	3.6	1
12	Barriers to predictive high-throughput screening for spin-crossover. *Computational Materials Science*, **2022**, 206, 111161	3.2	1
11	High-throughput density functional calculations to optimize properties and interfacial chemistry of piezoelectric materials. *Physical Review Materials*, **2018**, 2,	3.2	1
10	Split-vacancy defect complexes of oxygen in hcp and fcc cobalt. *Physical Review Materials*, **2020**, 4,	3.2	1

9	Remarkable low-energy properties of the pseudogapped semimetal Be5Pt. *Physical Review B*, **2020**, 102,	3.3	1
8	Strain modulation using defects in two-dimensional MoS2. *Physical Review B*, **2020**, 102,	3.3	1
7	Computational synthesis of substrates by crystal cleavage. *Npj Computational Materials*, **2021**, 7,	10.9	1
6	Physically and chemically smooth cesium-antimonide photocathodes on single crystal strontium titanate substrates. *Applied Physics Letters*, **2022**, 120, 194102	3.4	1
5	Accuracy of Quantum Monte Carlo Methods for Point Defects in Solids **2011**, 17-31		
4	Applying for computational time on NSF's TeraGrid, the world's largest cyberinfrastructure supporting open research. *Jom*, **2010**, 62, 17-18	2.1	
3	Large-Scale Molecular Dynamics Simulations of Interstitial Defect Diffusion in Silicon. *Materials Research Society Symposia Proceedings*, **2002**, 731, 9101		
2	Fundamental Cluster and Hydrogen Sites in Ti-Zr-Ni Quasicrystals. *Materials Research Society Symposia Proceedings*, **2000**, 643, 521		
1	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	