Richard G Hennig

List of Publications by Year
in descending order

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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	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
2	Machine learning of superconducting critical temperature from Eliashberg theory. Npj Computational Materials, 2022, 8, .	3.5	27
3	Ligand Optimization of Exchange Interaction in Co(II) Dimer Single Molecule Magnet by Machine Learning. Journal of Physical Chemistry A, 2022, 126, 529-535.	1.1	2
4	Limitations of empirical supercell extrapolation for calculations of point defects in bulk, at surfaces, and in two-dimensional materials. Physical Review B, 2022, 105, .	1.1	6
5	Barriers to predictive high-throughput screening for spin-crossover. Computational Materials Science, 2022, 206, 111161.	1.4	9
6	Giant Stokes shift for charged vacancies in monolayer SnS. Physical Review Materials, 2022, 6, .	0.9	2
7	Photoluminescence Induced by Substitutional Nitrogen in Single-Layer Tungsten Disulfide. ACS Nano, 2022, 16, 7428-7437.	7.3	7
8	Physically and chemically smooth cesium-antimonide photocathodes on single crystal strontium titanate substrates. Applied Physics Letters, 2022, 120, .	1.5	5
9	Synthesis of borophane polymorphs through hydrogenation of borophene. Science, 2021, 371, 1143-1148.	6.0	129
10	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.	0.7	0
11	Controllable pâ€Type Doping of 2D WSe₂ via Vanadium Substitution. Advanced Functional Materials, 2021, 31, 2105252.	7.8	40
12	High-pressure study of the low- Z rich superconductor Be22Re. Physical Review B, 2021, 104, .	1.1	2
13	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, .	1.1	4
14	Computational synthesis of substrates by crystal cleavage. Npj Computational Materials, 2021, 7, .	3.5	2
15	Charged vacancy defects in monolayer phosphorene. Physical Review Materials, 2021, 5, .	0.9	5
16	Experimental investigation of the Alâ€“Coâ€“Fe phase diagram over the whole composition range. Journal of Alloys and Compounds, 2020, 815, 152110.	2.8	12
17	New experimental studies on the phase diagram of the Al-Cu-Fe quasicrystal-forming system. Materials and Design, 2020, 185, 108186.	3.3	17
18	Phase equilibria and diffusion coefficients in the Fe-Zn binary system. Materials and Design, 2020, 188, 108437.	3.3	7

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19	Remarkable low-energy properties of the pseudogapped semimetal Be5Pt. Physical Review B, 2020, 102, .	1.1	1
20	Augmenting machine learning of energy landscapes with local structural information. Journal of Applied Physics, 2020, 128, .	1.1	13
21	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, .	1.1	8
22	Scalable Substitutional Reâ€Doping and its Impact on the Optical and Electronic Properties of Tungsten Diselenide. Advanced Materials, 2020, 32, e2005159.	11.1	32
23	Controlling neutral and charged excitons in MoS₂ with defects. Journal of Materials Research, 2020, 35, 949-957.	1.2	12
24	Machine learning of octahedral tilting in oxide perovskites by symbolic classification with compressed sensing. Computational Materials Science, 2020, 180, 109690.	1.4	19
25	Role of magnetism on transition metal oxide surfaces in vacuum and solvent. Physical Review Materials, 2020, 4, .	0.9	5
26	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, .	0.9	24
27	Split-vacancy defect complexes of oxygen in hcp and fcc cobalt. Physical Review Materials, 2020, 4, .	0.9	1
28	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, .	0.9	9
29	Multi-objective optimization of interatomic potentials with application to MgO. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 074007.	0.8	7
30	Functional form of the superconducting critical temperature from machine learning. Physical Review B, 2019, 100, .	1.1	35
31	Implicit self-consistent electrolyte model in plane-wave density-functional theory. Journal of Chemical Physics, 2019, 151, 234101.	1.2	561
32	The Conundrum of Relaxation Volumes in First-Principles Calculations of Charged Defects in UO2. Applied Sciences (Switzerland), 2019, 9, 5276.	1.3	11
33	Nanocrystal Symmetry Breaking and Accelerated Solid-State Diffusion in the Leadâ€“Cadmium Sulfide Cation Exchange system. Chemistry of Materials, 2019, 31, 991-1005.	3.2	16
34	Machine learning of ab-initio energy landscapes for crystal structure predictions. Computational Materials Science, 2019, 158, 414-419.	1.4	14
35	Predicting the Electrochemical Synthesis of 2D Materials from First Principles. Journal of Physical Chemistry C, 2019, 123, 3180-3187.	1.5	34
36	Insights into the Charge-Transfer Stabilization of Heterostructure Components with Unstable Bulk Analogs. Chemistry of Materials, 2018, 30, 4738-4747.	3.2	12

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37	Candidate replacements for lead in CH3NH3PbI3 from first principles calculations. Computational Materials Science, 2018, 155, 69-73.	1.4	7
38	High-throughput density functional calculations to optimize properties and interfacial chemistry of piezoelectric materials. Physical Review Materials, 2018, 2, .	0.9	4
39	Topology-Scaling Identification of Layered Solids and Stable Exfoliated 2D Materials. Physical Review Letters, 2017, 118, 106101.	2.9	262
40	Evaluation and comparison of classical interatomic potentials through a user-friendly interactive web-interface. Scientific Data, 2017, 4, 160125.	2.4	18
41	Pressure-induced superconductivity in the giant Rashba system BiTeI. Journal of Physics Condensed Matter, 2017, 29, 09LT02.	0.7	11
42	Exploring Periodic Bicontinuous Cubic Network Structures with Complete Phononic Bandgaps. Journal of Physical Chemistry C, 2017, 121, 22347-22352.	1.5	24
43	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></ Physical Review B, 2017, 96, .	1.1	63
44	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.	4.0	93
45	Interfaceâ€Driven Structural Distortions and Composition Segregation in Twoâ€Dimensional Heterostructures. Angewandte Chemie - International Edition, 2017, 56, 14448-14452.	7.2	8
46	Two-Dimensional Intrinsic Half-Metals With Large Spin Gaps. Nano Letters, 2017, 17, 5251-5257.	4.5	172
47	Computational methods for 2D materials: discovery, property characterization, and application design. Journal of Physics Condensed Matter, 2017, 29, 473001.	0.7	55
48	Interfaceâ€Driven Structural Distortions and Composition Segregation in Twoâ€Dimensional Heterostructures. Angewandte Chemie, 2017, 129, 14640-14644.	1.6	1
49	Genetic algorithm prediction of two-dimensional group-IV dioxides for dielectrics. Physical Review B, 2017, 95, .	1.1	23
50	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:msub> monolayers and bilayers. Physical Review B, 2017, 96, .	1.1	91
51	Role of composition and structure on the properties of metal/multifunctional ceramic interfaces. Journal of Applied Physics, 2016, 120, .	1.1	6
52	Computational characterization of lightweight multilayer MXene Li-ion battery anodes. Applied Physics Letters, 2016, 108, .	1.5	79
53	Computational discovery and characterization of polymorphic two-dimensional IVâ€“V materials. Applied Physics Letters, 2016, 109, .	1.5	60
54	Properties of Ti/TiC Interfaces from Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2016, 120, 12530-12538.	1.5	25

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55	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.	7.3	16
56	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:msub></mml:mrow></mml:math> Physical Review B, 2016, 94, .	3.7	75
57	Grand-canonical evolutionary algorithm for the prediction of two-dimensional materials. Physical Review B, 2016, 93, .	3.7	59
58	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> Physical Review B, 2016, 93, .	3.7	209
59	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, .	3.7	176
60	MPInterfaces: A Materials Project based Python tool for high-throughput computational screening of interfacial systems. Computational Materials Science, 2016, 122, 183-190.	1.4	95
61	Dynamical properties of AlN nanostructures and heterogeneous interfaces predicted using COMB potentials. Computational Materials Science, 2016, 113, 80-87.	1.4	23
62	Enhanced Liâ€“S Batteries Using Amine-Functionalized Carbon Nanotubes in the Cathode. ACS Nano, 2016, 10, 1050-1059.	7.3	289
63	Predicted Surface Composition and Thermodynamic Stability of MXenes in Solution. Journal of Physical Chemistry C, 2016, 120, 3550-3556.	1.5	196
64	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
65	Rashba effect in single-layer antimony telluroiodide SbTeI. Physical Review B, 2015, 92, .	3.7	60
66	Computational discovery of lanthanide doped and Co-doped Y3Al5O12 for optoelectronic applications. Applied Physics Letters, 2015, 107, 112109.	3.3	10
67	Comparison of polynomial approximations to speed up planewave-based quantum Monte Carlo calculations. Journal of Computational Physics, 2015, 287, 77-87.	1.9	2
68	Computational Screening of 2D Materials for Photocatalysis. Journal of Physical Chemistry Letters, 2015, 6, 1087-1098.	2.1	641
69	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.	1.2	103
70	Strong spin-lattice coupling in CrSiTe3. APL Materials, 2015, 3, .	2.2	192
71	Ab initiostudies of Cs on GaAs (100) and (110) surfaces. Physical Review B, 2015, 91, .	3.7	14
72	Al2O3 as a suitable substrate and a dielectric layer for n-layer MoS2. Applied Physics Letters, 2015, 107, 053106.	3.3	30

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73	Ab Initio Prediction of Piezoelectricity in Two-Dimensional Materials. ACS Nano, 2015, 9, 9885-9891.	7.3	445
74	Hybrid cathode architectures for lithium batteries based on TiS₂ and sulfur. Journal of Materials Chemistry A, 2015, 3, 19857-19866.	5.2	119
75	High throughput screening of substrates for synthesis and functionalization of 2D materials. Proceedings of SPIE, 2015, , .	0.8	3
76	ReaxFF molecular dynamics simulations on lithiated sulfur cathode materials. Physical Chemistry Chemical Physics, 2015, 17, 3383-3393.	1.3	143
77	Ab initio prediction of the Li5Ge2 Zintl compound. Computational Materials Science, 2014, 93, 133-136.	1.4	8
78	Importance of high-angular-momentum channels in pseudopotentials for quantum Monte Carlo. Physical Review B, 2014, 90, .	1.1	8
79	Computational prediction and characterization of single-layer CrS₂. Applied Physics Letters, 2014, 104, 022116.	1.5	108
80	Tethered Molecular Sorbents: Enabling Metalâ€Sulfur Battery Cathodes. Advanced Energy Materials, 2014, 4, 1400390.	10.2	67
81	Computational Discovery, Characterization, and Design of Single-Layer Materials. Jom, 2014, 66, 366-374.	0.9	41
82	Implicit solvation model for density-functional study of nanocrystal surfaces and reaction pathways. Journal of Chemical Physics, 2014, 140, 084106.	1.2	1,676
83	Structure and Stability Prediction of Compounds with Evolutionary Algorithms. Topics in Current Chemistry, 2014, 345, 181-222.	4.0	31
84	Computational synthesis of single-layer GaN on refractory materials. Applied Physics Letters, 2014, 105, .	1.5	46
85	Solidâ€“Solid Phase Transformations Induced through Cation Exchange and Strain in 2D Heterostructured Copper Sulfide Nanocrystals. Nano Letters, 2014, 14, 7090-7099.	4.5	147
86	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.	7.3	12
87	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.	1.5	91
88	Computational prediction of two-dimensional group-IV mono-chalcogenides. Applied Physics Letters, 2014, 105, .	1.5	245
89	Ab initiosynthesis of single-layer III-V materials. Physical Review B, 2014, 89, .	1.1	112
90	The Nanocrystal Superlattice Pressure Cell: A Novel Approach To Study Molecular Bundles under Uniaxial Compression. Nano Letters, 2014, 14, 4763-4766.	4.5	9

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91	Single-Layer Group-III Monochalcogenide Photocatalysts for Water Splitting. Chemistry of Materials, 2013, 25, 3232-3238.	3.2	675
92	Computational Search for Single-Layer Transition-Metal Dichalcogenide Photocatalysts. Journal of Physical Chemistry C, 2013, 117, 20440-20445.	1.5	468
93	(NH4)2S, a highly reactive molecular precursor for low temperature anion exchange reactions in nanoparticles. Dalton Transactions, 2013, 42, 12596.	1.6	33
94	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, .	1.1	215
95	Computational identification of single-layer CdO for electronic and optical applications. Applied Physics Letters, 2013, 103, .	1.5	52
96	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.	0.7	52
97	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
98	Li-Carboxylate Anode Structure-Property Relationships from Molecular Modeling. Chemistry of Materials, 2013, 25, 132-141.	3.2	75
99	Computational discovery of single-layer III-V materials. Physical Review B, 2013, 87, .	1.1	318
100	Structures, phase stabilities, and electrical potentials of Li-Si battery anode materials. Physical Review B, 2013, 87, .	1.1	41
101	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.	1.5	128
102	Accuracy of exchange-correlation functionals and effect of solvation on the surface energy of copper. Physical Review B, 2013, 87, .	1.1	211
103	Scaling relation for thermal ripples in single and multilayer graphene. Physical Review B, 2013, 87, .	1.1	25
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	Electronic structures of single-layer boron pnictides. Applied Physics Letters, 2012, 101, .	1.5	114
106	Synchrotron x-ray spectroscopy studies of valence and magnetic state in europium metal to extreme pressures. Physical Review B, 2012, 85, .	1.1	20
107	Unintended Phosphorus Doping of Nickel Nanoparticles during Synthesis with TOP: A Discovery through Structural Analysis. Nano Letters, 2012, 12, 4530-4539.	4.5	81
108	Framework for solvation in quantum Monte Carlo. Physical Review B, 2012, 85, .	1.1	14

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109	Ab initioprediction of environmental embrittlement at a crack tip in aluminum. Physical Review B, 2012, 86, .	1.1	34
110	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.	7.8	10
111	Predicting Nanocrystal Shape through Consideration of Surface-Ligand Interactions. ACS Nano, 2012, 6, 2118-2127.	7.3	236
112	Angle-Resolved Raman Imaging of Interlayer Rotations and Interactions in Twisted Bilayer Graphene. Nano Letters, 2012, 12, 3162-3167.	4.5	299
113	Predicting Chiral Nanostructures, Lattices and Superlattices in Complex Multicomponent Nanoparticle Self-Assembly. Nano Letters, 2012, 12, 3218-3223.	4.5	24
114	Tailored redox functionality of small organics for pseudocapacitive electrodes. Energy and Environmental Science, 2012, 5, 7176.	15.6	58
115	Ab initiobased empirical potential used to study the mechanical properties of molybdenum. Physical Review B, 2012, 85, .	1.1	71
116	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
117	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
118	Pressure-induced structural transitions in europium to 92 GPa. Physical Review B, 2011, 83, .	1.1	33
119	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
120	Softened Elastic Response and Unzipping in Chemical Vapor Deposition Graphene Membranes. Nano Letters, 2011, 11, 2259-2263.	4.5	316
121	Coupled quantumâ€“continuum analysis of crack tip processes in aluminum. Journal of the Mechanics and Physics of Solids, 2011, 59, 2476-2487.	2.3	20
122	Accuracy of quantum Monte Carlo methods for point defects in solids. Physica Status Solidi (B): Basic Research, 2011, 248, 267-274.	0.7	34
123	Energy landscape of silicon tetraâ€interstitials using an optimized classical potential. Physica Status Solidi (B): Basic Research, 2011, 248, 2050-2055.	0.7	14
124	Back Cover: Accuracy of quantum Monte Carlo methods for point defects in solids (Phys. Status) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 1	0.7	0
125	Spectroscopic Characterization of Charged Defects in Polycrystalline Pentacene by Timeâ€and Wavelengthâ€Resolved Electric Force Microscopy. Advanced Materials, 2011, 23, 624-628.	11.1	26
126	Threeâ€Dimensionally Isotropic Negative Refractive Index Materials from Block Copolymer Selfâ€Assembled Chiral Gyroid Networks. Angewandte Chemie - International Edition, 2011, 50, 11985-11989.	7.2	116

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127	Silver delafossite nitride, AgTaN2?. Journal of Solid State Chemistry, 2011, 184, 7-11.	1.4	17
128	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, .	1.1	12
129	Applying for computational time on NSFâ€™s TeraGridâ€”the worldâ€™s largest cyberinfrastructure supporting open research. Jom, 2010, 62, 17-18.	0.9	0
130	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, .	1.1	65
131	Mesoscopic structure prediction of nanoparticle assembly and coassembly: Theoretical foundation. Journal of Chemical Physics, 2010, 133, 194108.	1.2	26
132	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
133	Phase Behavior of Pseudobinary Precious Metalâ“Carbide Systems. Journal of Physical Chemistry C, 2010, 114, 21664-21671.	1.5	5
134	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.	1.5	21
135	Emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys. Nature, 2008, 451, 445-448.	13.7	111
136	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>Î‰</mml:mi></mml:math>titanium phases. Physical Review B, 2008, 78, .	1.1	173
137	Quantum Monte Carlo algorithms for electronic structure at the petascale; the Endstation project. Journal of Physics: Conference Series, 2008, 125, 012057.	0.3	24
138	Questioning the existence of a unique ground-state structure for Si clusters. Physical Review B, 2007, 75, .	1.1	62
139	Alleviation of the Fermion-Sign Problem by Optimization of Many-Body Wave Functions. Physical Review Letters, 2007, 98, 110201.	2.9	411
140	From compact point defects to extended structures in silicon. European Physical Journal B, 2007, 57, 229-234.	0.6	15
141	Empirical tight-binding model for titanium phase transformations. Physical Review B, 2006, 73, .	1.1	30
142	Location and energy of interstitial hydrogen in the1â^•1approximantW-TiZrNiof the icosahedralTiZrNiquasicrystal: Rietveld refinement of x-ray and neutron diffraction data and density-functional calculations. Physical Review B, 2006, 73, .	1.1	7
143	Hydrogen storage in Tiâ€“Zr and Tiâ€“Hf-based quasicrystals. Philosophical Magazine, 2006, 86, 957-964.	0.7	39
144	Diffusion mechanisms for silicon di-interstitials. Physical Review B, 2006, 73, .	1.1	9

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145	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
146	Ab initioTi-Zr-Ni phase diagram predicts stability of icosahedral TiZrNi quasicrystals. Physical Review B, 2005, 71, .	1.1	29
147	Impurities block the Î± to ï‰ martensitic transformation in titanium. Nature Materials, 2005, 4, 129-133.	13.3	207
148	Systematic pathway generation and sorting in martensitic transformations: TitaniumÎ±toï‰. Physical Review B, 2005, 72, .	1.1	27
149	Fast diffusion mechanism of silicon tri-interstitial defects. Physical Review B, 2005, 72, .	1.1	11
150	Complexity of Small Silicon Self-Interstitial Defects. Physical Review Letters, 2004, 92, 045501.	2.9	69
151	New Mechanism for theÎ±toï‰Martensitic Transformation in Pure Titanium. Physical Review Letters, 2003, 91, 025701.	2.9	156
152	Structure of the icosahedral Ti-Zr-Ni quasicrystal. Physical Review B, 2003, 67, .	1.1	46
153	Rietveld refinement and ab initio calculations of a C14-like Laves phase in Ti-Zr-Ni. Philosophical Magazine Letters, 2003, 83, 65-71.	0.5	9
154	Large-Scale Molecular Dynamics Simulations of Interstitial Defect Diffusion in Silicon. Materials Research Society Symposia Proceedings, 2002, 731, 9101.	0.1	0
155	Electronic structure of dangling bonds in amorphous silicon studied via a density-matrix functional method. Physical Review B, 2002, 66, .	1.1	10
156	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.	2.8	16
157	Ab-initio Study of the Ground-State Phase Diagram of the Icosahedral Ti-Zr-Ni Quasicrystal. Springer Proceedings in Physics, 2002, , 204-208.	0.1	0
158	Density-matrix functional method for electronic properties of impurities. Physical Review B, 2001, 63, .	1.1	19
159	Fundamental Cluster and Hydrogen Sites in Ti-Zr-Ni Quasicrystals. Materials Research Society Symposia Proceedings, 2000, 643, 521.	0.1	0
160	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.	0.8	16