Paul R C Kent

List of Publications by Year
in descending order

178 papers	31,995 citations	26567 56 h-index	4628 170 g-index
179 all docs	179 docs citations	179 times ranked	32635 citing authors

#	Article	IF	Citations
1	Geant4â€"a simulation toolkit. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2003, 506, 250-303.	0.7	17,893
2	Two-Dimensional, Ordered, Double Transition Metals Carbides (MXenes). ACS Nano, 2015, 9, 9507-9516.	7.3	1,395
3	Role of Surface Structure on Li-Ion Energy Storage Capacity of Two-Dimensional Transition-Metal Carbides. Journal of the American Chemical Society, 2014, 136, 6385-6394.	6.6	1,164
4	Prediction and Characterization of MXene Nanosheet Anodes for Non-Lithium-Ion Batteries. ACS Nano, 2014, 8, 9606-9615.	7.3	814
5	Atomic Defects in Monolayer Titanium Carbide (Ti₃C₂T_x) MXene. ACS Nano, 2016, 10, 9193-9200.	7.3	785
6	Hybrid density functional study of structural and electronic properties of functionalized Ti<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow		

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19	Multimodality of Structural, Electrical, and Gravimetric Responses of Intercalated MXenes to Water. ACS Nano, 2017, 11, 11118-11126.	7.3	183
20	Computational Insights into Materials and Interfaces for Capacitive Energy Storage. Advanced Science, 2017, 4, 1700059.	5.6	176
21	Competitive lithium solvation of linear and cyclic carbonates from quantum chemistry. Physical Chemistry Chemical Physics, 2016, 18, 164-175.	1.3	165
22	Understanding the origin of high-rate intercalation pseudocapacitance in Nb2O5 crystals. Journal of Materials Chemistry A, 2013, 1, 14951.	5.2	134
23	In situ atomistic insight into the growth mechanisms of single layer 2D transition metal carbides. Nature Communications, 2018, 9, 2266.	5.8	125
24	Criteria for Predicting the Formation of Single-Phase High-Entropy Alloys. Physical Review X, 2015, 5, .	2.8	123
25	Competing antiferromagnetism in a quasi-2D itinerant ferromagnet: Fe ₃ GeTe ₂. 2D Materials, 2017, 4, 011005.	2.0	123
26	Binding and Diffusion of Lithium in Graphite: Quantum Monte Carlo Benchmarks and Validation of van der Waals Density Functional Methods. Journal of Chemical Theory and Computation, 2014, 10, 5318-5323.	2.3	117
27	Nanoscale Elastic Changes in 2D Ti₃C₂T_x (MXene) Pseudocapacitive Electrodes. Advanced Energy Materials, 2016, 6, 1502290.	10.2	117
28	Accurate Static and Dynamic Properties of Liquid Electrolytes for Li-Ion Batteries from ab initio Molecular Dynamics. Journal of Physical Chemistry B, 2011, 115, 3085-3090.	1.2	115
29	Pseudogap and Antiferromagnetic Correlations in the Hubbard Model. Physical Review Letters, 2006, 97, 036401.	2.9	111
30	Solidâ€“Electrolyte Interphase Formation and Electrolyte Reduction at Li-Ion Battery Graphite Anodes: Insights from First-Principles Molecular Dynamics. Journal of Physical Chemistry C, 2012, 116, 24476-24481.	1.5	111
31	Computational Discovery and Design of MXenes for Energy Applications: Status, Successes, and Opportunities. ACS Applied Materials & Interfaces, 2019, 11, 24885-24905.	4.0	105
32	Tracking ion intercalation into layered Ti₃C₂ MXene films across length scales. Energy and Environmental Science, 2020, 13, 2549-2558.	15.6	100
33	Finite-size errors in quantum many-body simulations of extended systems. Physical Review B, 1999, 59, 1917-1929.	1.1	98
34	Anomalous Lattice Dynamics near the Ferroelectric Instability in PbTe. Physical Review Letters, 2011, 107, 175503.	2.9	97
35	Phonon softening and metallization of a narrow-gap semiconductor by thermal disorder. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 4725-4730.	3.3	96
36	Understanding controls on interfacial wetting at epitaxial graphene: Experiment and theory. Physical Review B, 2012, 85, .	1.1	95

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37	Monte Carlo energy and variance-minimization techniques for optimizing many-body wave functions. Physical Review B, 1999, 59, 12344-12351.	1.1	94
38	Carrier localization and the origin of luminescence in cubic InGaN alloys. Applied Physics Letters, 2001, 79, 1977-1979.	1.5	94
39	Itinerant Antiferromagnetism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>RuO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review Letters, 2017, 118, 077201.	2.9	89
40	Double transition metal MXenes with wide band gaps and novel magnetic properties. Nanoscale, 2018, 10, 11962-11968.	2.8	88
41	Quantum Monte Carlo Study of the Optical and Diffusive Properties of the Vacancy Defect in Diamond. Physical Review Letters, 2003, 91, 076403.	2.9	84
42	Carbon clusters near the crossover to fullerene stability. Physical Review B, 2000, 62, 15394-15397.	1.1	83
43	Neutral and charged excitations in carbon fullerenes from first-principles many-body theories. Journal of Chemical Physics, 2008, 129, 084311.	1.2	83
44	Novel Cooperative Interactions and Structural Ordering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Let	2.9	80
45	QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. Journal of Chemical Physics, 2020, 152, 174105.	1.2	80
46	Effects of Surface Terminations of 2D Bi₂WO₆ on Photocatalytic Hydrogen Evolution from Water Splitting. ACS Applied Materials & Interfaces, 2020, 12, 20067-20074.	4.0	78
47	Pseudopotential theory of dilute IIIÂV nitrides. Semiconductor Science and Technology, 2002, 17, 851-859.	1.0	76
48	Hydrogen Bonds and Vibrations of Water on (110) Rutile. Journal of Physical Chemistry C, 2009, 113, 13732-13740.	1.5	74
49	Charge-order fluctuations in one-dimensional silicides. Nature Materials, 2008, 7, 539-542.	13.3	70
50	Computational Screening of MXene Electrodes for Pseudocapacitive Energy Storage. Journal of Physical Chemistry C, 2019, 123, 315-321.	1.5	69
51	Efficient calculation of the antiferromagnetic phase diagram of the three-dimensional Hubbard model. Physical Review B, 2005, 72, .	1.1	67
52	Origin of Nanoscale Phase Stability Reversals in Titanium Oxide Polymorphs. Journal of Physical Chemistry C, 2009, 113, 4240-4245.	1.5	62
53	Ab initioQuantum MonteÂCarlo Calculations of Spin Superexchange in Cuprates: The Benchmarking Case of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ca</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review X, 2014, 4, .	2.8	61
54	Rashba effect in single-layer antimony telluroiodide SbTeI. Physical Review B, 2015, 92, .	1.1	60

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55	Solvent-type-dependent polymorphism and charge transport in a long fused-ring organic semiconductor. Nanoscale, 2014, 6, 449-456.	2.8	59
56	Reactive Force Field Study of Li/C Systems for Electrical Energy Storage. Journal of Chemical Theory and Computation, 2015, 11, 2156-2166.	2.3	59
57	Phase stability of TiO₂polymorphs from diffusion Quantum Monte Carlo. New Journal of Physics, 2016, 18, 113049.	1.2	59
58	Edge Segregated Polymorphism in 2D Molybdenum Carbide. Advanced Materials, 2019, 31, e1808343.	11.1	56
59	Structural stability and defect energetics of ZnO from diffusion quantum Monte Carlo. Journal of Chemical Physics, 2015, 142, 164705.	1.2	55
60	Surface Reorganization Leads to Enhanced Photocatalytic Activity in Defective BiOCl. Chemistry of Materials, 2018, 30, 5128-5136.	3.2	55
61	Microstructure and a Nucleation Mechanism for Nanoprecipitates inPbTeâˆ’AgSbTe2. Physical Review Letters, 2009, 103, 145502.	2.9	54
62	Formation, characterization, and dynamics of onion-like carbon structures for electrical energy storage from nanodiamonds using reactive force fields. Journal of Applied Physics, 2011, 110, .	1.1	53
63	Interfacial and electronic properties of heterostructures of MXene and graphene. Physical Review B, 2019, 99, .	1.1	53
64	Proton Redox and Transport in MXene-Confined Water. ACS Applied Materials & Interfaces, 2020, 12, 763-770.	4.0	53
65	Exascale applications: skin in the game. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190056.	1.6	53
66	Li-ion site disorder driven superionic conductivity in solid electrolytes: a first-principles investigation of Î²-Li₃PS₄. Journal of Materials Chemistry A, 2017, 5, 1153-1159.	5.2	50
67	Atomistic description of the electronic structure ofInxGa1âˆ’xAsalloys and InAs/GaAs superlattices. Physical Review B, 2002, 66, .	1.1	49
68	Biaxial strain-modified valence and conduction band offsets of zinc-blende GaN, GaP, GaAs, InN, InP, and InAs, and optical bowing of strained epitaxial InGaN alloys. Applied Physics Letters, 2002, 81, 4377-4379.	1.5	48
69	Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2014, 118, 16236-16245.	1.5	48
70	Vibrational Density of States of Strongly H-Bonded Interfacial Water: Insights from Inelastic Neutron Scattering and Theory. Journal of Physical Chemistry C, 2014, 118, 10805-10813.	1.5	48
71	Oxygen vacancy diffusion in bulk SrTiO3 from density functional theory calculations. Computational Materials Science, 2016, 118, 309-315.	1.4	48
72	Combined density functional and dynamical cluster quantum Monte Carlo calculations of the three-band Hubbard model for hole-doped cuprate superconductors. Physical Review B, 2008, 78, .	1.1	47

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73	Comment on â€œStructure and dynamics of liquid water on rutile TiO2(110)â€• Physical Review B, 2012, 85, .	1.1	46
74	Toward a predictive theory of correlated materials. Science, 2018, 361, 348-354.	6.0	45
75	How Water Attacks MXene. Chemistry of Materials, 2022, 34, 4975-4982.	3.2	44
76	Accuracy of ab initio electron correlation and electron densities in vanadium dioxide. Physical Review Materials, 2017, 1, .	0.9	41
77	Quantum Monte Carlo calculations of the one-body density matrix and excitation energies of silicon. Physical Review B, 1998, 57, 15293-15302.	1.1	39
78	Diffusion quantum Monte Carlo study of the equation of state and point defects in aluminum. Physical Review B, 2012, 85, .	1.1	38
79	A Novel and Functional Single-Layer Sheet of ZnSe. ACS Applied Materials & Interfaces, 2015, 7, 1458-1464.	4.0	38
80	Structureâ€“activity relationship of Au/ZrO2 catalyst on formation of hydroxyl groups and its influence on CO oxidation. Journal of Materials Chemistry A, 2013, 1, 6051.	5.2	36
81	Cohesive energy and structural parameters of binary oxides of groups IIA and IIIB from diffusion quantum Monte Carlo. Journal of Chemical Physics, 2016, 144, 174707.	1.2	36
82	Improved treatment of exact exchange in Quantum ESPRESSO. Computer Physics Communications, 2017, 214, 52-58.	3.0	36
83	Electronic properties of doped and defective NiO: A quantum Monte Carlo study. Physical Review Materials, 2017, 1, .	0.9	36
84	Role of Hydroxyl Groups on the Stability and Catalytic Activity of Au Clusters on a Rutile Surface. Journal of Physical Chemistry Letters, 2011, 2, 2918-2924.	2.1	35
85	Multiscale and Multimodal Characterization of 2D Titanium Carbonitride MXene. Advanced Materials Interfaces, 2020, 7, 1902207.	1.9	35
86	Faster proton transfer dynamics of water on SnO2 compared to TiO2. Journal of Chemical Physics, 2011, 134, 044706.	1.2	34
87	Failure of nitrogen cluster states to emerge into the bandgap of GaAsN with application of pressure. Applied Physics Letters, 2003, 82, 559-561.	1.5	33
88	Modeling Water Adsorption on Rutile (110) Using van der Waals Density Functional and DFT+U Methods. Journal of Physical Chemistry C, 2013, 117, 23638-23644.	1.5	33
89	Electronic Structure of xDNA. Journal of Physical Chemistry B, 2007, 111, 9057-9061.	1.2	31
90	A comparative study of surface energies and water adsorption on Ce-bastnÃsite, La-bastnÃsite, and calcite via density functional theory and water adsorption calorimetry. Physical Chemistry Chemical Physics, 2017, 19, 7820-7832.	1.3	30

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91	Crystal Structures, Surface Stability, and Water Adsorption Energies of La-BastnÃsite via Density Functional Theory and Experimental Studies. Journal of Physical Chemistry C, 2016, 120, 16767-16781.	1.5	28
92	Pseudopotentials for correlated-electron calculations. Physical Review B, 2000, 62, 13347-13355.	1.1	27
93	Detection of hydrogen using graphene. Nanoscale Research Letters, 2012, 7, 198.	3.1	27
94	Quantum Monte Carlo analysis of a charge ordered insulating antiferromagnet: the Ti₄O₇ MagnÃ©li phase. Physical Chemistry Chemical Physics, 2016, 18, 18323-18335.	1.3	27
95	Diffusion quantum Monte Carlo calculations of SrFeO3 and LaFeO3. Journal of Chemical Physics, 2017, 147, 034701.	1.2	27
96	Structures, Energetics, and Electronic Properties of Layered Materials and Nanotubes of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2013, 117, 25817-25825.	1.5	26
97	Tuning from Half-Metallic to Semiconducting Behavior in SiC Nanoribbons. Journal of Physical Chemistry C, 2013, 117, 15447-15455.	1.5	26
98	Understanding the interactions between oxygen vacancies atSrTiO3(001) surfaces. Physical Review B, 2014, 90, .	1.1	26
99	Effects of partial La filling and Sb vacancy defects on <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>CoS</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> skutterudites. Physical Review B, 2017, 95, .	1.1	26
100	Nitrogen pairs, triplets, and clusters in GaAs and GaP. Applied Physics Letters, 2001, 79, 2339-2341.	1.5	25
101	Self-healing diffusion quantum Monte Carlo algorithms: Direct reduction of the fermion sign error in electronic structure calculations. Physical Review B, 2009, 79, .	1.1	25
102	Quantum Monte Carlo algorithms for electronic structure at the petascale; the Endstation project. Journal of Physics: Conference Series, 2008, 125, 012057.	0.3	24
103	Systematic Reduction of Sign Errors in Many-Body Calculations of Atoms and Molecules. Physical Review Letters, 2010, 104, 193001.	2.9	24
104	Metalâ€“insulator transition tuned by oxygen vacancy migration across TiO2/VO2 interface. Scientific Reports, 2020, 10, 18554.	1.6	24
105	Rapid Diagnosis of Nonconvulsive Status Epilepticus Using Reduced-Lead Electroencephalography. Western Journal of Emergency Medicine, 2015, 16, 442-446.	0.6	23
106	Coupling of Acetaldehyde to Crotonaldehyde on CeO_{2â€“x}(111): Bifunctional Mechanism and Role of Oxygen Vacancies. Journal of Physical Chemistry C, 2019, 123, 8273-8286.	1.5	23
107	A fast and efficient algorithm for Slater determinant updates in quantum Monte Carlo simulations. Journal of Chemical Physics, 2009, 130, 204105.	1.2	22
108	Successes and failures of Hubbard-corrected density functional theory: The case of Mg doped LiCoO2. Journal of Chemical Physics, 2014, 141, 164706.	1.2	22

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109	Doping a bad metal: Origin of suppression of the metal-insulator transition in nonstoichiometric <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>VO</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2020, 101, .	1.1	21
110	Intercalationâ€Induced Reversible Electrochromic Behavior of Twoâ€Dimensional Ti₃C₂T_x MXene in Organic Electrolytes. ChemElectroChem, 2021, 8, 151-156.	1.7	21
111	Evaluating and Optimizing the NERSC Workload on Knights Landing. , 2016, , .		20
112	Development and performance of a mixed OpenMP/MPI quantum Monte Carlo code. Concurrency and Computation: Practice and Experience, 2000, 12, 1121-1129.	0.6	19
113	Epitaxial Stabilization of Ferromagnetism in the Nanophase of FeGe. Physical Review Letters, 2006, 96, 127201.	2.9	19
114	Computational challenges of large-scale, long-time, first-principles molecular dynamics. Journal of Physics: Conference Series, 2008, 125, 012058.	0.3	19
115	Structure of YSi2 nanowires from scanning tunneling spectroscopy and first principles. Applied Physics Letters, 2009, 95, 123107.	1.5	19
116	Role of Polytetrahedral Structures in the Elongation and Rupture of Gold Nanowires. ACS Nano, 2011, 5, 10065-10073.	7.3	18
117	Nanodopant-Induced Band Modulation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>AgPb</mml:mi><mml:mi>m</mml:mi></mml:msub><mml:msub><mml:mi>SbTe</mml:mi><mml:mi><m Thermoelectrics. Physical Review Letters, 2011, 106, 206601.	2.9	18
118	Density Functional Theory Study of Oxygen Reduction Activity on Ultrathin Platinum Nanotubes. Journal of Physical Chemistry C, 2012, 116, 16499-16510.	1.5	18
119	Single-Site and Monolayer Surface Hydration Energy of Anatase and Rutile Nanoparticles Using Density Functional Theory. Journal of Physical Chemistry C, 2013, 117, 26084-26090.	1.5	18
120	Magnitude of pseudopotential localization errors in fixed node diffusion quantum Monte Carlo. Journal of Chemical Physics, 2017, 146, 244101.	1.2	18
121	Self-diffusion of Ti interstitial based point defects and complexes in TiC. Acta Materialia, 2019, 165, 381-387.	3.8	18
122	Doped NiO: The mottness of a charge transfer insulator. Physical Review B, 2020, 101, .	1.1	16
123	Optimized structure and electronic band gap of monolayer GeSe from quantum Monte Carlo methods. Physical Review Materials, 2021, 5, .	0.9	16
124	Toward a systematic improvement of the fixed-node approximation in diffusion Monte Carlo for solidsâ€”A case study in diamond. Journal of Chemical Physics, 2020, 153, 184111.	1.2	16
125	The effects of annealing on the structural, optical, and vibrational properties of lattice-matched GaAsSbNâˆ•GaAs grown by molecular beam epitaxy. Journal of Applied Physics, 2007, 102, 023503.	1.1	15
126	Effects of N incorporation on the structural and photoluminescence characteristics of GaSbN/GaSb single quantum wells. Journal of Applied Physics, 2007, 101, 113508.	1.1	15

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127	Structure and growth of quasi-one-dimensional YSi₂nanophases on Si(100). Journal of Physics Condensed Matter, 2013, 25, 014011.	0.7	15
128	Diffusion Monte Carlo: A pathway towards an accurate theoretical description of manganese oxides. Physical Review Materials, 2018, 2, .	0.9	15
129	Interfacial charge transfer and interaction in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mrow><mml:mi>MXene</mml:mi><mml:mo>/</mml:mo><mml:mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> heterostructures. Physical Review Materials, 2021, 5, .	0.9	14
130	OpenMP application experiences: Porting to accelerated nodes. Parallel Computing, 2022, 109, 102856.	1.3	14
131	Penetration of electronic perturbations of dilute nitrogen impurities deep into the conduction band ofGaP1â^'xNx. Physical Review B, 2004, 70, .	1.1	13
132	Quantum Monte Carlo calculations of dihydrogen binding energetics on Ca cations: An assessment of errors in density functionals for weakly bonded systems. Physical Review B, 2010, 82, .	1.1	13
133	Spin-resolved self-doping tunes the intrinsic half-metallicity of AlN nanoribbons. Nano Research, 2014, 7, 63-70.	5.8	13
134	Systematic comparison and cross-validation of fixed-node diffusion Monte Carlo and phaseless auxiliary-field quantum Monte Carlo in solids. Physical Review B, 2020, 102, .	1.1	13
135	Perspectives on van der Waals Density Functionals: The Case of TiS₂. Journal of Physical Chemistry A, 2020, 124, 9867-9876.	1.1	13
136	Origin of metal-insulator transitions in correlated perovskite metals. Physical Review Research, 2022, 4, .	1.3	13
137	Density-density functionals and effective potentials in many-body electronic structure calculations. Physical Review B, 2008, 77, .	1.1	12
138	Quantum Monte Carlo calculations for ground and excited states. International Journal of Quantum Chemistry, 2002, 86, 218-225.	1.0	11
139	van der Waals forces: Accurate calculation and assessment of approximate methods in dielectric nanocolloids up to 16 nm. Journal of Chemical Physics, 2009, 131, 144705.	1.2	11
140	Geochemical reaction mechanism discovery from molecular simulation. Environmental Chemistry, 2015, 12, 20.	0.7	11
141	Grain boundary stability and influence on ionic conductivity in a disordered perovskiteâ€"a first-principles investigation of lithium lanthanum titanate. MRS Communications, 2016, 6, 455-463.	0.8	11
142	Combining configurational energies and forces for molecular force field optimization. Journal of Chemical Physics, 2017, 147, 161713.	1.2	11
143	Gaussian process based optimization of molecular geometries using statistically sampled energy surfaces from quantum Monte Carlo. Journal of Chemical Physics, 2018, 149, 164116.	1.2	10
144	Hybrid DFT investigation of the energetics of Mg ion diffusion in Î±-MoO₃. Physical Chemistry Chemical Physics, 2018, 20, 24877-24884.	1.3	10

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145	Fast Rotational Diffusion of Water Molecules in a 2D Hydrogen Bond Network at Cryogenic Temperatures. Physical Review Letters, 2018, 120, 196001.	2.9	10
146	A combined machine learning and density functional theory study of binary Ti-Nb and Ti-Zr alloys: Stability and Youngâ€™s modulus. Computational Materials Science, 2020, 184, 109830.	1.4	10
147	Intrinsic low thermal conductivity in weakly ionic rocksalt structures. Physical Review B, 2015, 92, .	1.1	9
148	Investigating the Accuracy of Water Models through the Van Hove Correlation Function. Journal of Chemical Theory and Computation, 2021, 17, 5992-6005.	2.3	9
149	Oxygen vacancy formation energies in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>PbTiO</mml:mi><mml:mn>3</mml:mn><mml:mi></mml:mi></mml:msub></mml:mrow></mml:math> superlattice. Physical Review Materials, 2018, 2, .	3.1	8
150	Density Functional Study of the Structure, Stability and Oxygen Reduction Activity of Ultrathin Platinum Nanowires. Journal of the Electrochemical Society, 2013, 160, F548-F553.	1.3	7
151	Quantum Many-Body Effects in Defective Transition-Metal-Oxide Superlattices. Journal of Chemical Theory and Computation, 2017, 13, 5604-5609.	2.3	7
152	Atomic Defects and Edge Structure in Single-layer Ti₃C₂T_x MXene. Microscopy and Microanalysis, 2017, 23, 1704-1705.	0.2	7
153	Delayed Slater determinant update algorithms for high efficiency quantum Monte Carlo. Journal of Chemical Physics, 2017, 147, 174107.	1.2	7
154	Compton profile of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>VO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml across the metal-insulator transition: Evidence of a non-Fermi liquid metal. Physical Review B, 2019, 99, .	1.1	7
155	The correlation between N deficiency and the mechanical properties of the Ti2AlNy MAX phase. Journal of the European Ceramic Society, 2020, 40, 2279-2286.	2.8	7
156	Surrogate Hessian accelerated structural optimization for stochastic electronic structure theories. Journal of Chemical Physics, 2022, 156, 054104.	1.2	7
157	Tunable one-dimensional electron gas carrier densities at nanostructured oxide interfaces. Scientific Reports, 2016, 6, 25452.	1.6	6
158	An efficient hybrid orbital representation for quantum Monte Carlo calculations. Journal of Chemical Physics, 2018, 149, 084107.	1.2	6
159	Local structure of potassium doped nickel oxide: A combined experimental-theoretical study. Physical Review Materials, 2019, 3, .	0.9	6
160	Ferromagnetism and carrier polarization of Mn-doped II-IV-V2 chalcopyrites. AIP Conference Proceedings, 2005, , .	0.3	4
161	Polaronic Transport and Current Blockades in Epitaxial Silicide Nanowires and Nanowire Arrays. Nano Letters, 2013, 13, 3684-3689.	4.5	4
162	Trustworthy predictions. Nature, 2013, 493, 314-315.	13.7	4

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163	Dynamic load balancing for petascale quantum Monte Carlo applications: The Alias method. Computer Physics Communications, 2013, 184, 284-292.	3.0	4
164	Novel boron nitride MXenes as promising energy storage materials. Nanoscale, 2022, 14, 9086-9096.	2.8	4
165	Dimensional control of defect dynamics in perovskite oxide superlattices. Physical Review Materials, 2018, 2, .	0.9	3
166	Electron and Hole Confinement in GaInN/GaN and AlGaN/GaN Quantum Wells. Materials Research Society Symposia Proceedings, 2001, 693, 63.	0.1	2
167	Evolution of Electron States with Composition in GaAsN Alloys. Physica Status Solidi (B): Basic Research, 2001, 228, 253-257.	0.7	2
168	New algorithm to enable 400+ TFlop/s sustained performance in simulations of disorder effects in high-T<inf>c</inf> superconductors. , 2008, , .		2
169	Simple impurity embedded in a spherical jellium: Approximations of density functional theory compared to quantum Monte Carlo benchmarks. Physical Review B, 2011, 84, .	1.1	2
170	Delayed Update Algorithms for Quantum Monte Carlo Simulation on GPU. , 2016, , .		2
171	Optimal Linear Water Density for Proton Transport in Tunnel Oxides. Journal of Physical Chemistry C, 2021, 125, 11508-11512.	1.5	2
172	Improved hydrocarbon potentials for sputtering studies. Journal of Nuclear Materials, 2011, 415, S183-S186.	1.3	1
173	Development of QMCPACK for Exascale Scientific Computing. , 2017, , 461-480.		1
174	New insights into high temperature superconductivity from a computational solution of the two-dimensional Hubbard model. Journal of Physics: Conference Series, 2005, 16, 257-268.	0.3	0
175	Publisher's Note: Efficient calculation of the antiferromagnetic phase diagram of the three-dimensional Hubbard model [Phys. Rev. B72, 060411 (2005)]. Physical Review B, 2005, 72, .	1.1	0
176	Theoretical Study of the Structure, Stability and Oxygen Reduction Activity of Ultrathin Platinum Nanowires. ECS Transactions, 2013, 50, 1385-1395.	0.3	0
177	Atomic Electron Tomography: Probing 3D Structure and Material Properties at the Single-Atom Level. Microscopy and Microanalysis, 2017, 23, 1886-1887.	0.2	0
178	Atomic Electron Tomography: Adding a New Dimension to See Single Atoms in Materials. Microscopy and Microanalysis, 2018, 24, 558-559.	0.2	0