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	OpenMP application experiences: Porting to accelerated nodes. Parallel Computing, 2022, 109, 102856.	1.3	14
2	Surrogate Hessian accelerated structural optimization for stochastic electronic structure theories. Journal of Chemical Physics, 2022, 156, 054104.	1.2	7
3	Origin of metal-insulator transitions in correlated perovskite metals. Physical Review Research, 2022, 4, .	1.3	13
4	How Water Attacks MXene. Chemistry of Materials, 2022, 34, 4975-4982.	3.2	44
5	Novel boron nitride MXenes as promising energy storage materials. Nanoscale, 2022, 14, 9086-9096.	2.8	4
6	Intercalationâ€Induced Reversible Electrochromic Behavior of Twoâ€Dimensional Ti₃C₂T_x MXene in Organic Electrolytes. ChemElectroChem, 2021, 8, 151-156.	1.7	21
7	Optimized structure and electronic band gap of monolayer GeSe from quantum Monte Carlo methods. Physical Review Materials, 2021, 5, .	0.9	16
8	Optimal Linear Water Density for Proton Transport in Tunnel Oxides. Journal of Physical Chemistry C, 2021, 125, 11508-11512.	1.5	2
9	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
10	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
11	Proton Redox and Transport in MXene-Confined Water. ACS Applied Materials & Interfaces, 2020, 12, 763-770.	4.0	53
12	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
13	Perspectives on van der Waals Density Functionals: The Case of TiS₂. Journal of Physical Chemistry A, 2020, 124, 9867-9876.	1.1	13
14	Metalâ€“insulator transition tuned by oxygen vacancy migration across TiO2/VO2 interface. Scientific Reports, 2020, 10, 18554.	1.6	24
15	Exascale applications: skin in the game. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190056.	1.6	53
16	Doped NiO: The mottness of a charge transfer insulator. Physical Review B, 2020, 101, .	1.1	16
17	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
18	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

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19	Tracking ion intercalation into layered Ti₃C₂ MXene films across length scales. Energy and Environmental Science, 2020, 13, 2549-2558.	15.6	100
20	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
21	Multiscale and Multimodal Characterization of 2D Titanium Carbonitride MXene. Advanced Materials Interfaces, 2020, 7, 1902207.	1.9	35
22	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></mml Physical Review B, 2020, 101, .	1.1	21
23	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
24	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
25	Computational Discovery and Design of MXenes for Energy Applications: Status, Successes, and Opportunities. ACS Applied Materials & Interfaces, 2019, 11, 24885-24905.	4.0	105
26	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
27	Edge Segregated Polymorphism in 2D Molybdenum Carbide. Advanced Materials, 2019, 31, e1808343.	11.1	56
28	Interfacial and electronic properties of heterostructures of MXene and graphene. Physical Review B, 2019, 99, .	1.1	53
29	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
30	Computational Screening of MXene Electrodes for Pseudocapacitive Energy Storage. Journal of Physical Chemistry C, 2019, 123, 315-321.	1.5	69
31	Self-diffusion of Ti interstitial based point defects and complexes in TiC. Acta Materialia, 2019, 165, 381-387.	3.8	18
32	Local structure of potassium doped nickel oxide: A combined experimental-theoretical study. Physical Review Materials, 2019, 3, .	0.9	6
33	Understanding the MXene Pseudocapacitance. Journal of Physical Chemistry Letters, 2018, 9, 1223-1228.	2.1	231
34	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
35	Hybrid DFT investigation of the energetics of Mg ion diffusion in Î±-MoO₃. Physical Chemistry Chemical Physics, 2018, 20, 24877-24884.	1.3	10
36	Atomic Electron Tomography: Adding a New Dimension to See Single Atoms in Materials. Microscopy and Microanalysis, 2018, 24, 558-559.	0.2	0

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37	An efficient hybrid orbital representation for quantum Monte Carlo calculations. Journal of Chemical Physics, 2018, 149, 084107.	1.2	6
38	<tt>QMCPACK</tt>: an open sourceab initioquantum Monte Carlo package for the electronic structure of atoms, molecules and solids. Journal of Physics Condensed Matter, 2018, 30, 195901.	0.7	187
39	Toward a predictive theory of correlated materials. Science, 2018, 361, 348-354.	6.0	45
40	Surface Reorganization Leads to Enhanced Photocatalytic Activity in Defective BiOCl. Chemistry of Materials, 2018, 30, 5128-5136.	3.2	55
41	Fast Rotational Diffusion of Water Molecules in a 2D Hydrogen Bond Network at Cryogenic Temperatures. Physical Review Letters, 2018, 120, 196001.	2.9	10
42	In situ atomistic insight into the growth mechanisms of single layer 2D transition metal carbides. Nature Communications, 2018, 9, 2266.	5.8	125
43	Double transition metal MXenes with wide band gaps and novel magnetic properties. Nanoscale, 2018, 10, 11962-11968.	2.8	88
44	Dimensional control of defect dynamics in perovskite oxide superlattices. Physical Review Materials, 2018, 2, .	0.9	3
45	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><m superlattice. Physical Review Materials, 2018, 2, .	0.9	8
46	Diffusion Monte Carlo: A pathway towards an accurate theoretical description of manganese oxides. Physical Review Materials, 2018, 2, .	0.9	15
47	Deciphering chemical order/disorder and material properties at the single-atom level. Nature, 2017, 542, 75-79.	13.7	243
48	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
49	Improved treatment of exact exchange in Quantum ESPRESSO. Computer Physics Communications, 2017, 214, 52-58.	3.0	36
50	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 Physical Review Letters, 2017, 118, 077201.	2.9	89
51	Computational Insights into Materials and Interfaces for Capacitive Energy Storage. Advanced Science, 2017, 4, 1700059.	5.6	176
52	Magnitude of pseudopotential localization errors in fixed node diffusion quantum Monte Carlo. Journal of Chemical Physics, 2017, 146, 244101.	1.2	18
53	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
54	Competing antiferromagnetism in a quasi-2D itinerant ferromagnet: Fe ₃ GeTe ₂. 2D Materials, 2017, 4, 011005.	2.0	123

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55	Multimodality of Structural, Electrical, and Gravimetric Responses of Intercalated MXenes to Water. ACS Nano, 2017, 11, 11118-11126.	7.3	183
56	Quantum Many-Body Effects in Defective Transition-Metal-Oxide Superlattices. Journal of Chemical Theory and Computation, 2017, 13, 5604-5609.	2.3	7
57	Diffusion quantum Monte Carlo calculations of SrFeO3 and LaFeO3. Journal of Chemical Physics, 2017, 147, 034701.	1.2	27
58	Atomic Defects and Edge Structure in Single-layer Ti₃C₂T_x MXene. Microscopy and Microanalysis, 2017, 23, 1704-1705.	0.2	7
59	Delayed Slater determinant update algorithms for high efficiency quantum Monte Carlo. Journal of Chemical Physics, 2017, 147, 174107.	1.2	7
60	Combining configurational energies and forces for molecular force field optimization. Journal of Chemical Physics, 2017, 147, 161713.	1.2	11
61	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
62	Atomic Electron Tomography: Probing 3D Structure and Material Properties at the Single-Atom Level. Microscopy and Microanalysis, 2017, 23, 1886-1887.	0.2	0
63	Accuracy of ab initio electron correlation and electron densities in vanadium dioxide. Physical Review Materials, 2017, 1, .	0.9	41
64	Electronic properties of doped and defective NiO: A quantum Monte Carlo study. Physical Review Materials, 2017, 1, .	0.9	36
65	Development of QMCPACK for Exascale Scientific Computing. , 2017, , 461-480.		1
66	Evaluating and Optimizing the NERSC Workload on Knights Landing. , 2016, , .		20
67	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
68	Phase stability of TiO₂polymorphs from diffusion Quantum Monte Carlo. New Journal of Physics, 2016, 18, 113049.	1.2	59
69	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
70	Oxygen vacancy diffusion in bulk SrTiO3 from density functional theory calculations. Computational Materials Science, 2016, 118, 309-315.	1.4	48
71	Atomic Defects in Monolayer Titanium Carbide (Ti₃C₂T_x) MXene. ACS Nano, 2016, 10, 9193-9200.	7.3	785
72	Delayed Update Algorithms for Quantum Monte Carlo Simulation on GPU. , 2016, , .		2

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73	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
74	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, .	3.1	299
75	Tunable one-dimensional electron gas carrier densities at nanostructured oxide interfaces. Scientific Reports, 2016, 6, 25452.	1.6	6
76	Nanoscale Elastic Changes in 2D Ti₃C₂T_x (MXene) Pseudocapacitive Electrodes. Advanced Energy Materials, 2016, 6, 1502290.	10.2	117
77	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
78	Competitive lithium solvation of linear and cyclic carbonates from quantum chemistry. Physical Chemistry Chemical Physics, 2016, 18, 164-175.	1.3	165
79	Effect of Metal Ion Intercalation on the Structure of MXene and Water Dynamics on its Internal Surfaces. ACS Applied Materials & Interfaces, 2016, 8, 8859-8863.	4.0	225
80	Control of electronic properties of 2D carbides (MXenes) by manipulating their transition metal layers. Nanoscale Horizons, 2016, 1, 227-234.	4.1	394
81	Ultrathin nanosheets of CrSiTe₃: a semiconducting two-dimensional ferromagnetic material. Journal of Materials Chemistry C, 2016, 4, 315-322.	2.7	235
82	Intrinsic low thermal conductivity in weakly ionic rocksalt structures. Physical Review B, 2015, 92, .	1.1	9
83	Rashba effect in single-layer antimony telluroiodide SbTeI. Physical Review B, 2015, 92, .	1.1	60
84	Rapid Diagnosis of Nonconvulsive Status Epilepticus Using Reduced-Lead Electroencephalography. Western Journal of Emergency Medicine, 2015, 16, 442-446.	0.6	23
85	A Novel and Functional Single-Layer Sheet of ZnSe. ACS Applied Materials & Interfaces, 2015, 7, 1458-1464.	4.0	38
86	Two-Dimensional, Ordered, Double Transition Metals Carbides (MXenes). ACS Nano, 2015, 9, 9507-9516.	7.3	1,395
87	Structural stability and defect energetics of ZnO from diffusion quantum Monte Carlo. Journal of Chemical Physics, 2015, 142, 164705.	1.2	55
88	Computational discovery of ferromagnetic semiconducting single-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrSnTe</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Physical Review B, 2015, 92, .	1.1	212
89	Criteria for Predicting the Formation of Single-Phase High-Entropy Alloys. Physical Review X, 2015, 5, .	2.8	123
90	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

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91	Geochemical reaction mechanism discovery from molecular simulation. Environmental Chemistry, 2015, 12, 20.	0.7	11
92	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:mi>Cu</mml:mi></mml:mrow><mml:msub><mml:mrow><mml:mi>O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review X, 2014, 4, .	2.8	61
93	Understanding the interactions between oxygen vacancies atSrTiO3(001) surfaces. Physical Review B, 2014, 90, .	1.1	26
94	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
95	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
96	Theoretical Predictions of Freestanding Honeycomb Sheets of Cadmium Chalcogenides. Journal of Physical Chemistry C, 2014, 118, 16236-16245.	1.5	48
97	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
98	Prediction and Characterization of MXene Nanosheet Anodes for Non-Lithium-Ion Batteries. ACS Nano, 2014, 8, 9606-9615.	7.3	814
99	Spin-resolved self-doping tunes the intrinsic half-metallicity of AlN nanoribbons. Nano Research, 2014, 7, 63-70.	5.8	13
100	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
101	Solvent-type-dependent polymorphism and charge transport in a long fused-ring organic semiconductor. Nanoscale, 2014, 6, 449-456.	2.8	59
102	Understanding the origin of high-rate intercalation pseudocapacitance in Nb2O5 crystals. Journal of Materials Chemistry A, 2013, 1, 14951.	5.2	134
103	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
104	Polaronic Transport and Current Blockades in Epitaxial Silicide Nanowires and Nanowire Arrays. Nano Letters, 2013, 13, 3684-3689.	4.5	4
105	Trustworthy predictions. Nature, 2013, 493, 314-315.	13.7	4
106	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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109	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
110	Tuning from Half-Metallic to Semiconducting Behavior in SiC Nanoribbons. Journal of Physical Chemistry C, 2013, 117, 15447-15455.	1.5	26
111	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
112	Structure and growth of quasi-one-dimensional YSi₂nanophases on Si(100). Journal of Physics Condensed Matter, 2013, 25, 014011.	0.7	15
113	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
114	Theoretical Study of the Structure, Stability and Oxygen Reduction Activity of Ultrathin Platinum Nanowires. ECS Transactions, 2013, 50, 1385-1395.	0.3	0
115	Understanding controls on interfacial wetting at epitaxial graphene: Experiment and theory. Physical Review B, 2012, 85, .	1.1	95
116	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
117	Comment on â€œStructure and dynamics of liquid water on rutile TiO2(110)â€• Physical Review B, 2012, 85, .	1.1	46
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	Diffusion quantum Monte Carlo study of the equation of state and point defects in aluminum. Physical Review B, 2012, 85, .	1.1	38
120	Detection of hydrogen using graphene. Nanoscale Research Letters, 2012, 7, 198.	3.1	27
121	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
122	Role of Polytetrahedral Structures in the Elongation and Rupture of Gold Nanowires. ACS Nano, 2011, 5, 10065-10073.	7.3	18
123	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
124	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
125	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
126	Improved hydrocarbon potentials for sputtering studies. Journal of Nuclear Materials, 2011, 415, S183-S186.	1.3	1

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127	Faster proton transfer dynamics of water on SnO2 compared to TiO2. Journal of Chemical Physics, 2011, 134, 044706.	1.2	34
128	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><mm Thermoelectrics. Physical Review Letters, 2011, 106, 206601.	2.9	18
129	Anomalous Lattice Dynamics near the Ferroelectric Instability in PbTe. Physical Review Letters, 2011, 107, 175503.	2.9	97
130	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
131	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
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	Systematic Reduction of Sign Errors in Many-Body Calculations of Atoms and Molecules. Physical Review Letters, 2010, 104, 193001.	2.9	24
134	Microstructure and a Nucleation Mechanism for Nanoprecipitates inPbTeâ^'AgSbTe2. Physical Review Letters, 2009, 103, 145502.	2.9	54
135	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
136	Structure of YSi2 nanowires from scanning tunneling spectroscopy and first principles. Applied Physics Letters, 2009, 95, 123107.	1.5	19
137	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
138	A fast and efficient algorithm for Slater determinant updates in quantum Monte Carlo simulations. Journal of Chemical Physics, 2009, 130, 204105.	1.2	22
139	Hydrogen Bonds and Vibrations of Water on (110) Rutile. Journal of Physical Chemistry C, 2009, 113, 13732-13740.	1.5	74
140	Thermodynamic properties of PbTe, PbSe, and PbS: First-principles study. Physical Review B, 2009, 80, .	1.1	231
141	Origin of Nanoscale Phase Stability Reversals in Titanium Oxide Polymorphs. Journal of Physical Chemistry C, 2009, 113, 4240-4245.	1.5	62
142	Charge-order fluctuations in one-dimensional silicides. Nature Materials, 2008, 7, 539-542.	13.3	70
143	New algorithm to enable 400+ TFlop/s sustained performance in simulations of disorder effects in high-T<inf>c</inf> superconductors. , 2008, , .		2
144	Quantum Monte Carlo algorithms for electronic structure at the petascale; the Endstation project. Journal of Physics: Conference Series, 2008, 125, 012057.	0.3	24

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145	Neutral and charged excitations in carbon fullerenes from first-principles many-body theories. Journal of Chemical Physics, 2008, 129, 084311.	1.2	83
146	Density-density functionals and effective potentials in many-body electronic structure calculations. Physical Review B, 2008, 77, .	1.1	12
147	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
148	Computational challenges of large-scale, long-time, first-principles molecular dynamics. Journal of Physics: Conference Series, 2008, 125, 012058.	0.3	19
149	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
150	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
151	Electronic Structure of xDNA. Journal of Physical Chemistry B, 2007, 111, 9057-9061.	1.2	31
152	Pseudogap and Antiferromagnetic Correlations in the Hubbard Model. Physical Review Letters, 2006, 97, 036401.	2.9	111
153	Epitaxial Stabilization of Ferromagnetism in the Nanophase of FeGe. Physical Review Letters, 2006, 96, 127201.	2.9	19
154	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
155	Ferromagnetism and carrier polarization of Mn-doped II-IV-V2 chalcopyrites. AIP Conference Proceedings, 2005, , .	0.3	4
156	Systematic Study ofd-Wave Superconductivity in the 2D Repulsive Hubbard Model. Physical Review Letters, 2005, 95, 237001.	2.9	248
157	Efficient calculation of the antiferromagnetic phase diagram of the three-dimensional Hubbard model. Physical Review B, 2005, 72, .	1.1	67
158	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
159	Penetration of electronic perturbations of dilute nitrogen impurities deep into the conduction band ofGaP1âˆ’xNx. Physical Review B, 2004, 70, .	1.1	13
160	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
161	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
162	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

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163	Pseudopotential theory of dilute IIIÂV nitrides. Semiconductor Science and Technology, 2002, 17, 851-859.	1.0	76
164	Atomistic description of the electronic structure ofInxGa1â^'xAsalloys and InAs/GaAs superlattices. Physical Review B, 2002, 66, .	1.1	49
165	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
166	Quantum Monte Carlo calculations for ground and excited states. International Journal of Quantum Chemistry, 2002, 86, 218-225.	1.0	11
167	Evolution of III-V Nitride Alloy Electronic Structure: The Localized to Delocalized Transition. Physical Review Letters, 2001, 86, 2613-2616.	2.9	248
168	Theory of electronic structure evolution in GaAsN and GaPN alloys. Physical Review B, 2001, 64, .	1.1	385
169	Carrier localization and the origin of luminescence in cubic InGaN alloys. Applied Physics Letters, 2001, 79, 1977-1979.	1.5	94
170	Electron and Hole Confinement in GaInN/GaN and AlGaN/GaN Quantum Wells. Materials Research Society Symposia Proceedings, 2001, 693, 63.	0.1	2
171	Evolution of Electron States with Composition in GaAsN Alloys. Physica Status Solidi (B): Basic Research, 2001, 228, 253-257.	0.7	2
172	Nitrogen pairs, triplets, and clusters in GaAs and GaP. Applied Physics Letters, 2001, 79, 2339-2341.	1.5	25
173	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
174	Pseudopotentials for correlated-electron calculations. Physical Review B, 2000, 62, 13347-13355.	1.1	27
175	Carbon clusters near the crossover to fullerene stability. Physical Review B, 2000, 62, 15394-15397.	1.1	83
176	Finite-size errors in quantum many-body simulations of extended systems. Physical Review B, 1999, 59, 1917-1929.	1.1	98
177	Monte Carlo energy and variance-minimization techniques for optimizing many-body wave functions. Physical Review B, 1999, 59, 12344-12351.	1.1	94
178	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