David R Bowler

List of Publications by Year
in descending order

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115 papers	9,003 citations	147801 31 h-index	39675 94 g-index
143 all docs	143 docs citations	143 times ranked	11240 citing authors

#	Article	IF	Citations
1	Van der Waals density functionals applied to solids. Physical Review B, 2011, 83, .	3.2	3,608
2	Chemical accuracy for the van der Waals density functional. Journal of Physics Condensed Matter, 2010, 22, 022201.	1.8	2,222
3	mathcal{O}(N) methods in electronic structure calculations. Reports on Progress in Physics, 2012, 75, 036503.	20.1	432
4	Recent progress with large-scaleab initio calculations: the CONQUEST code. Physica Status Solidi (B): Basic Research, 2006, 243, 989-1000.	1.5	181
5	Gate controlling of quantum interference and direct observation of anti-resonances in single molecule charge transport. Nature Materials, 2019, 18, 357-363.	27.5	160
6	Calculations for millions of atoms with density functional theory: linear scaling shows its potential. Journal of Physics Condensed Matter, 2010, 22, 074207.	1.8	92
7	Self-assembled nanowires on semiconductor surfaces. Journal of Materials Science, 2006, 41, 4568-4603.	3.7	89
8	Beyond Ehrenfest: correlated non-adiabatic molecular dynamics. Journal of Physics Condensed Matter, 2004, 16, 8251-8266.	1.8	86
9	The transfer of energy between electrons and ions in solids. Reports on Progress in Physics, 2006, 69, 1195-1234.	20.1	77
10	Molecular conduction: Do time-dependent simulations tell you more than the Landauer approach?. Journal of Chemical Physics, 2006, 124, 214708.	3.0	75
11	Doping Nature of Native Defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mrow><m Physical Review Letters, 2014, 112, 197001.	7.8	71
12	Order-N first-principles calculations with the conquest code. Computer Physics Communications, 2007, 177, 14-18.	7.5	64
13	Dynamical simulation of inelastic quantum transport. Journal of Physics Condensed Matter, 2007, 19, 196201.	1.8	61
14	Correlated electronâ€“ion dynamics: the excitation of atomic motion by energetic electrons. Journal of Physics Condensed Matter, 2005, 17, 4793-4812.	1.8	57
15	Large scale and linear scaling DFT with the CONQUEST code. Journal of Chemical Physics, 2020, 152, 164112.	3.0	55
16	A critical assessment of theoretical methods for finding reaction pathways and transition states of surface processes. Journal of Physics Condensed Matter, 2010, 22, 074203.	1.8	54
17	Density matrices in O(N) electronic structure calculations: theory and applications. Computer Physics Communications, 1999, 120, 95-108.	7.5	52
18	Stripe and Short Range Order in the Charge Density Wave of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mrow><m Physical Review Letters, 2017, 118, 017002.	7.8	49

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19	Protonated Carboxyl Anchor for Stable Adsorption of Ru N749 Dye (Black Dye) on a TiO2 Anatase (101) Surface. Journal of Physical Chemistry Letters, 2012, 3, 472-477.	4.6	48
20	Short-range phase coherence and origin of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mo>â€</mml:m density wave. Physical Review B, 2016, 93, .	3.2	47
21	Adsorption of pentacene on a silicon surface. Surface Science, 2005, 578, 20-26.	1.9	45
22	Stable and Efficient Linear Scaling First-Principles Molecular Dynamics for 10000+ Atoms. Journal of Chemical Theory and Computation, 2014, 10, 5419-5425.	5.3	43
23	Parallel sparse matrix multiplication for linear scaling electronic structure calculations. Computer Physics Communications, 2001, 137, 255-273.	7.5	42
24	Adsorption of Thiophene-Conjugated Sensitizers on TiO₂ Anatase (101). Journal of Physical Chemistry C, 2010, 114, 20240-20248.	3.1	40
25	Understanding the role of ions and water molecules in the NaCl dissolution process. Journal of Chemical Physics, 2013, 139, 234702.	3.0	40
26	Atomic force algorithms in density functional theory electronic-structure techniques based on local orbitals. Journal of Chemical Physics, 2004, 121, 6186-6194.	3.0	39
27	Adsorption of Catechol on TiO₂ Rutile (100): A Density Functional Theory Investigation. Journal of Physical Chemistry C, 2010, 114, 6491-6495.	3.1	39
28	Interaction between electronic structure and strain in Bi nanolines on Si(001). Surface Science, 2003, 527, L177-L183.	1.9	36
29	Linear Scaling Constrained Density Functional Theory in CONQUEST. Journal of Chemical Theory and Computation, 2011, 7, 884-889.	5.3	36
30	Scanning tunneling microscopy of the charge density wave in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mo>â€</mml:m the presence of single atom defects. Physical Review B, 2015, 92, .	3.2	36
31	Molecular interactions and decomposition pathways ofNH3on Si(001). Physical Review B, 2007, 75, .	3.2	34
32	Pseudo-atomic orbitals as basis sets for the O(N) DFT code CONQUEST. Journal of Physics Condensed Matter, 2008, 20, 294206.	1.8	31
33	NH3on Si(001): Self-organized patterns of adsorbates investigated by a combination of scanning tunneling microscopy experiments and density functional theory calculations. Physical Review B, 2005, 72, .	3.2	29
34	Efficient Calculations with Multisite Local Orbitals in a Large-Scale DFT Code CONQUEST. Journal of Chemical Theory and Computation, 2014, 10, 4813-4822.	5.3	29
35	Local Real-Space View of the Achiral <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>â€</mml:mtext><mml:msub><mml:mrow><m <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>2</mml:mn><mml:mo>Ã—</mml:mo><mml:mrow><mml:mn>2</mml:mn><mml:mo>Ã—</m Physical Review Letters, 2018, 120, 136404.	7.8	29
36	Investigating individual arsenic dopant atoms in silicon using low-temperature scanning tunnelling microscopy. Journal of Physics Condensed Matter, 2014, 26, 012001.	1.8	28

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37	Structure of atomically perfect lines of bismuth in the Si(001) surface. Physical Review B, 2000, 62, 7237-7242.	3.2	27
38	Accuracy of order-Ndensity-functional theory calculations on DNA systems using CONQUEST. Journal of Physics Condensed Matter, 2008, 20, 294201.	1.8	25
39	Optimized multi-site local orbitals in the large-scale DFT program CONQUEST. Physical Chemistry Chemical Physics, 2015, 17, 31427-31433.	2.8	25
40	Effects of the Hubbard U on density functional-based predictions of BiFeO₃properties. Journal of Physics Condensed Matter, 2017, 29, 445501.	1.8	25
41	Insight into the Charge Density Wave Gap from Contrast Inversion in Topographic STM Images. Physical Review Letters, 2020, 125, 267603.	7.8	25
42	DSSC anchoring groups: a surface dependent decision. Journal of Physics Condensed Matter, 2014, 26, 195302.	1.8	24
43	A first principles study of sub-monolayer Ge on Si(). Surface Science, 2002, 515, 483-490.	1.9	23
44	Intrinsic Oxygen Vacancy and Extrinsic Aluminum Dopant Interplay: A Route to the Restoration of Defective TiO₂. Journal of Physical Chemistry C, 2014, 118, 7261-7271.	3.1	23
45	Encapsulation of atomic-scale Bi wires in epitaxial silicon without loss of structure. Physical Review B, 2005, 72, .	3.2	22
46	Electronic structure of Si(110)-(<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 studied by scanning tunneling spectroscopy and density functional theory. Physical Review B, 2011, 84, .	3.2	22
47	Large-scale DFT simulations with a linear-scaling DFT code CONQUEST on K-computer. Journal of Advanced Simulation in Science and Engineering, 2014, 1, 87-97.	0.2	22
48	Efficient Calculation of Electronic Structure Using O(N) Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 4146-4153.	5.3	21
49	Î" Self-Consistent Field Method for Natural Anthocyanidin Dyes. Journal of Chemical Theory and Computation, 2013, 9, 3181-3188.	5.3	19
50	Small polaron formation in dangling-bond wires on the Si(001) surface. Physical Review B, 2000, 63, .	3.2	18
51	The Energetics of Hut-Cluster Self-Assembly in Ge/Si(001) from Linear-Scaling DFT Calculations. Journal of the Physical Society of Japan, 2008, 77, 123706.	1.6	18
52	Density functional theory study of the iron-based porphyrin haem(b) on the Si(111):H surface. Physical Review B, 2009, 79, .	3.2	18
53	Effect of hydration of the TiO2 anatase (101) substrate on the atomic layer deposition of alumina films. Journal of Materials Chemistry, 2011, 21, 4197.	6.7	17
54	Linear scaling density matrix real time TDDFT: Propagator unitarity and matrix truncation. Journal of Chemical Physics, 2015, 143, 102801.	3.0	17

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55	Communication: Generalized canonical purification for density matrix minimization. Journal of Chemical Physics, 2016, 144, 091102.	3.0	17
56	Highly accurate local basis sets for large-scale DFT calculations in conquest. Japanese Journal of Applied Physics, 2019, 58, 100503.	1.5	17
57	Density functional calculations of Ge(105): Local basis sets andO(N)methods. Physical Review B, 2007, 76, .	3.2	16
58	Tight binding studies of strained Ge/Si() growth. Surface Science, 2003, 526, 356-366.	1.9	15
59	Local resilience of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>â^’</mm charge density wave to Ti self-doping. Physical Review B, 2017, 95, .	3.2	15
60	Correlated electronâ€“ion dynamics with open boundaries: formalism. Journal of Physics Condensed Matter, 2005, 17, 3985-3995.	1.8	14
61	Site-Dependent Ambipolar Charge States Induced by Group V Atoms in a Silicon Surface. ACS Nano, 2012, 6, 10456-10462.	14.6	14
62	Canonical-ensemble extended Lagrangian Bornâ€“Oppenheimer molecular dynamics for the linear scaling density functional theory. Journal of Physics Condensed Matter, 2017, 29, 405901.	1.8	14
63	Step structure of Si(110)-(16Ã—2)and adsorption ofH2O. Physical Review B, 2010, 82, .	3.2	13
64	Scalable Patterning of One-Dimensional Dangling Bond Rows on Hydrogenated Si(001). ACS Nano, 2013, 7, 4422-4428.	14.6	13
65	Non-self-consistent Density-Functional Theory Exchange-Correlation Forces for GGA Functionals. Journal of Chemical Theory and Computation, 2009, 5, 1499-1505.	5.3	12
66	Identification of intermediate linear structure formed during Bi/Si(001) surface anneal. Surface Science, 2005, 596, 163-175.	1.9	11
67	Electronic state of interstitial Cu in bulk Si: Density functional calculations. Physical Review B, 2006, 73, .	3.2	11
68	Atomic structure of misfit dislocations at InAs/GaAs(110). Journal of Physics Condensed Matter, 2008, 20, 235227.	1.8	11
69	Endotaxial Si nanolines in Si(001):H. Physical Review B, 2011, 84, .	3.2	11
70	Importance of bulk states for the electronic structure of semiconductor surfaces: implications for finite slabs. Journal of Physics Condensed Matter, 2017, 29, 145502.	1.8	11
71	Influence of crystal structure on charge carrier effective masses in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2019, 100, .	3.2	11
72	Polar Morphologies from First Principles: PbTiO₃ Films on SrTiO₃ Substrates and the p(2Ã—Î›) Surface Reconstruction. Advanced Theory and Simulations, 2020, 3, 2000154.	2.8	11

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73	Automatic data distribution and load balancing with space-filling curves: implementation in CONQUEST. Journal of Physics Condensed Matter, 2008, 20, 275223.	1.8	10
74	Density-functional theory study of gramicidin A ion channel geometry and electronic properties. Journal of the Royal Society Interface, 2013, 10, 20130547.	3.4	10
75	Linear-scaling first-principles molecular dynamics of complex biological systems with the Conquest code. Japanese Journal of Applied Physics, 2016, 55, 1102B1.	1.5	10
76	Exact location of dopants below the Si(001):H surface from scanning tunneling microscopy and density functional theory. Physical Review B, 2017, 95, .	3.2	10
77	High-accuracy large-scale DFT calculations using localized orbitals in complex electronic systems: the case of grapheneâ€“metal interfaces. Journal of Physics Condensed Matter, 2018, 30, 505901.	1.8	9
78	Ab initiostudy of subsurface diffusion of Cu on the H-passivated Si(001) surface. Physical Review B, 2009, 80, .	3.2	8
79	Si atom adsorption and diffusion on Si(110)-(1Ã—1)and(2Ã—1). Physical Review B, 2010, 81, .	3.2	8
80	H atom adsorption and diffusion on Si(110)-(1Ã—1) and (2Ã—1) surfaces. Physical Chemistry Chemical Physics, 2011, 13, 11367.	2.8	8
81	Coating TiO₂ Anatase by Amorphous Al₂O₃: Effects on Dyes Anchoring Through Carboxyl Groups. Journal of Physical Chemistry C, 2012, 116, 4408-4415.	3.1	8
82	Raoult's law revisited: accurately predicting equilibrium relative humidity points for humidity control experiments. Journal of Applied Crystallography, 2017, 50, 631-638.	4.5	8
83	Structural properties of siliconâ€“germanium and germaniumâ€“silicon coreâ€“shell nanowires. Journal of Physics Condensed Matter, 2018, 30, 465303.	1.8	8
84	1D semiconducting atomic chain of In and Bi on Si(001). Journal of Physics Condensed Matter, 2006, 18, L241-L249.	1.8	7
85	A density functional theory study of Mn nanowires on the Si(001) surface. Journal of Physics Condensed Matter, 2011, 23, 305003.	1.8	7
86	Blue moon ensemble simulation of aquation free energy profiles applied to mono and bifunctional platinum anticancer drugs. Journal of Computational Chemistry, 2020, 41, 1973-1984.	3.3	7
87	Model system for controlling strain in silicon at the atomic scale. Physical Review B, 2011, 84, .	3.2	6
88	Co-adsorption patterns of NH3 on Si(001): Comment on â€œThe ordering of the adsorbed NH3 molecules across the Si dimer rows on the Si(001) surfaceâ€. Surface Science, 2008, 602, 3760-3762.	1.9	5
89	Adsorption of phosphorus molecules evaporated from an InP solid source on the Si(100) surface. Physical Review B, 2013, 87, .	3.2	5
90	First-principles soft-mode lattice dynamics of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>PbZr</mml:mi><mml:mrow><mml:mn>0.5< mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and shortcomings of the virtual crystal approximation. Physical Review B, 2019, 100, .	3.2	5

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91	Short range and long range strain fields of Bi nanoline. Materials Science and Technology, 2004, 20, 955-958.	1.6	4
92	Comment on â€˜Bi nanolines on Si(001): registry with substrateâ€™. Nanotechnology, 2006, 17, 1801-1802.	2.6	4
93	Atomic-scale nanowires on Si(001): Cu on Bi. Physical Review B, 2010, 82, .	3.2	4
94	Non-adiabatic simulations of current-related structural transformations in metallic nanodevices. Journal of Physics Condensed Matter, 2011, 23, 345301.	1.8	4
95	Bi on the Si(001) surface. Physical Review B, 2012, 86, .	3.2	4
96	Atomic layer doping of Mn magnetic impurities from surface chains at a Ge/Si hetero-interface. Nanoscale, 2018, 10, 295-301.	5.6	4
97	Notes on density matrix perturbation theory. Journal of Chemical Physics, 2020, 153, 164105.	3.0	4
98	DFT study of undoped and As-doped Si nanowires approaching the bulk limit. Journal of Physics Condensed Matter, 2020, 32, 035304.	1.8	4
99	Dopant activation mechanism of Bi wire-Î´-doping into Si crystal, investigated with wavelength dispersive fluorescence x-ray absorption fine structure and density functional theory. Journal of Physics Condensed Matter, 2017, 29, 155001.	1.8	3
100	Alane adsorption and dissociation on the Si(0â€‰0â€‰1) surface. Journal of Physics Condensed Matter, 2017, 29, 395001.	1.8	3
101	Group V dimers on Si(001): Can they act as Lewis bases?. Surface Science, 2005, 595, 233-238.	1.9	2
102	Hydrogen adsorption and diffusion around Si(0â€‰0â€‰1)/Si(1â€‰1â€‰0) corners in nanostructures. Journal of Physics Condensed Matter, 2014, 26, 295301.	1.8	2
103	Subatomic electronic feature from dynamic motion of Si dimer defects in Bi nanolines on Si(001). Physical Review B, 2017, 96, .	3.2	2
104	Electronic coupling between Bi nanolines and the Si(001) substrate: An experimental and theoretical study. Physical Review B, 2017, 96, .	3.2	2
105	Towards surface diffusion potential mapping on atomic length scale. Journal of Applied Physics, 2019, 125, 184301.	2.5	2
106	The pseudoatomic orbital basis: electronic accuracy and soft-mode distortions in ABO₃ perovskites. Electronic Structure, 2020, 2, 025002.	2.8	2
107	Origin of Ferroelectric Domain Wall Alignment with Surface Trenches in Ultrathin Films. Physical Review Letters, 2021, 127, 247601.	7.8	2
108	Reaction paths of alane dissociation on the Si(0â€‰0â€‰1) surface. Journal of Physics Condensed Matter, 2018, 30, 105002.	1.8	1

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109	Planning a Project. , 2013, , 147-164.		0
110	Molecular Dynamics and Monte Carlo. , 2013, , 75-88.		0
111	Density Functional Theory in Detail. , 2013, , 127-143.		0
112	Building bridges: matching density functional theory with experiment. Contemporary Physics, 2018, 59, 377-390.	1.8	0
113	What to do with All the Numbers. , 0, , 235-252.		0
114	Coordinates and Simulation Cell. , 0, , 165-191.		0
115	Activation of two dopants, Bi and Er in Î´-doped layer in Si crystal. Nano Futures, 2021, 5, 045005.	2.2	0