David R Bowler

List of Publications by Year
in descending order

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	Activation of two dopants, Bi and Er in Î´-doped layer in Si crystal. Nano Futures, 2021, 5, 045005.	2.2	0
2	Origin of Ferroelectric Domain Wall Alignment with Surface Trenches in Ultrathin Films. Physical Review Letters, 2021, 127, 247601.	7.8	2
3	Notes on density matrix perturbation theory. Journal of Chemical Physics, 2020, 153, 164105.	3.0	4
4	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
5	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
6	Large scale and linear scaling DFT with the CONQUEST code. Journal of Chemical Physics, 2020, 152, 164112.	3.0	55
7	The pseudoatomic orbital basis: electronic accuracy and soft-mode distortions in ABO₃ perovskites. Electronic Structure, 2020, 2, 025002.	2.8	2
8	Insight into the Charge Density Wave Gap from Contrast Inversion in Topographic STM Images. Physical Review Letters, 2020, 125, 267603.	7.8	25
9	DFT study of undoped and As-doped Si nanowires approaching the bulk limit. Journal of Physics Condensed Matter, 2020, 32, 035304.	1.8	4
10	Towards surface diffusion potential mapping on atomic length scale. Journal of Applied Physics, 2019, 125, 184301.	2.5	2
11	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
12	Highly accurate local basis sets for large-scale DFT calculations in conquest. Japanese Journal of Applied Physics, 2019, 58, 100503.	1.5	17
13	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
14	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
15	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
16	Reaction paths of alane dissociation on the Si(0â€‰0â€‰1) surface. Journal of Physics Condensed Matter, 2018, 30, 105002.	1.8	1
17	Atomic layer doping of Mn magnetic impurities from surface chains at a Ge/Si hetero-interface. Nanoscale, 2018, 10, 295-301.	5.6	4
18	Building bridges: matching density functional theory with experiment. Contemporary Physics, 2018, 59, 377-390.	1.8	0

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19	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
20	Structural properties of siliconâ€“germanium and germaniumâ€“silicon coreâ€“shell nanowires. Journal of Physics Condensed Matter, 2018, 30, 465303.	1.8	8
21	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
22	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:mo>â€²</mml:mo></mml:mrow></mml:math> charge density wave to Ti self-doping. Physical Review B, 2017, 95, .	3.2	15
23	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
24	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:mo>â€²</mml:mo></mml:mrow></mml:math> Physical Review Letters, 2017, 118, 017002.	7.8	49
25	Effects of the Hubbard U on density functional-based predictions of BiFeO₃properties. Journal of Physics Condensed Matter, 2017, 29, 445501.	1.8	25
26	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
27	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
28	Subatomic electronic feature from dynamic motion of Si dimer defects in Bi nanolines on Si(001). Physical Review B, 2017, 96, .	3.2	2
29	Efficient Calculation of Electronic Structure Using O(N) Density Functional Theory. Journal of Chemical Theory and Computation, 2017, 13, 4146-4153.	5.3	21
30	Electronic coupling between Bi nanolines and the Si(001) substrate: An experimental and theoretical study. Physical Review B, 2017, 96, .	3.2	2
31	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
32	Alane adsorption and dissociation on the Si(0â€‰0â€‰1) surface. Journal of Physics Condensed Matter, 2017, 29, 395001.	1.8	3
33	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
34	Communication: Generalized canonical purification for density matrix minimization. Journal of Chemical Physics, 2016, 144, 091102.	3.0	17
35	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€²</mml:mo></mml:mrow></mml:math> density wave. Physical Review B, 2016, 93, .	3.2	17
36	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€²</mml:mo></mml:mrow></mml:math> the presence of single atom defects. Physical Review B, 2015, 92, .	3.2	36

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37	Linear scaling density matrix real time TDDFT: Propagator unitarity and matrix truncation. Journal of Chemical Physics, 2015, 143, 102801.	3.0	17
38	Optimized multi-site local orbitals in the large-scale DFT program CONQUEST. Physical Chemistry Chemical Physics, 2015, 17, 31427-31433.	2.8	25
39	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
40	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
41	DSSC anchoring groups: a surface dependent decision. Journal of Physics Condensed Matter, 2014, 26, 195302.	1.8	24
42	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
43	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
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	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
46	Investigating individual arsenic dopant atoms in silicon using low-temperature scanning tunnelling microscopy. Journal of Physics Condensed Matter, 2014, 26, 012001.	1.8	28
47	Planning a Project. , 2013, , 147-164.		0
48	Molecular Dynamics and Monte Carlo. , 2013, , 75-88.		0
49	Scalable Patterning of One-Dimensional Dangling Bond Rows on Hydrogenated Si(001). ACS Nano, 2013, 7, 4422-4428.	14.6	13
50	Density Functional Theory in Detail. , 2013, , 127-143.		0
51	Î” Self-Consistent Field Method for Natural Anthocyanidin Dyes. Journal of Chemical Theory and Computation, 2013, 9, 3181-3188.	5.3	19
52	Understanding the role of ions and water molecules in the NaCl dissolution process. Journal of Chemical Physics, 2013, 139, 234702.	3.0	40
53	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
54	Adsorption of phosphorus molecules evaporated from an InP solid source on the Si(100) surface. Physical Review B, 2013, 87, .	3.2	5

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55	Site-Dependent Ambipolar Charge States Induced by Group V Atoms in a Silicon Surface. ACS Nano, 2012, 6, 10456-10462.	14.6	14
56	Bi on the Si(001) surface. Physical Review B, 2012, 86, .	3.2	4
57	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
58	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
59	mathcal{O}(N) methods in electronic structure calculations. Reports on Progress in Physics, 2012, 75, 036503.	20.1	432
60	H atom adsorption and diffusion on Si(110)-(1Ã—1) and (2Ã—1) surfaces. Physical Chemistry Chemical Physics, 2011, 13, 11367.	2.8	8
61	Linear Scaling Constrained Density Functional Theory in CONQUEST. Journal of Chemical Theory and Computation, 2011, 7, 884-889.	5.3	36
62	A density functional theory study of Mn nanowires on the Si(001) surface. Journal of Physics Condensed Matter, 2011, 23, 305003.	1.8	7
63	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
64	Van der Waals density functionals applied to solids. Physical Review B, 2011, 83, .	3.2	3,608
65	Non-adiabatic simulations of current-related structural transformations in metallic nanodevices. Journal of Physics Condensed Matter, 2011, 23, 345301.	1.8	4
66	Model system for controlling strain in silicon at the atomic scale. Physical Review B, 2011, 84, .	3.2	6
67	Electronic structure of Si(110)-(<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML") Tj ETQq1 1 0.784314 rgBT /Overlo studied by scanning tunneling spectroscopy and density functional theory. Physical Review B, 2011, 84, .	3.2	22
68	Endotaxial Si nanolines in Si(001):H. Physical Review B, 2011, 84, .	3.2	11
69	Si atom adsorption and diffusion on Si(110)-(1Ã—1)and(2Ã—1). Physical Review B, 2010, 81, .	3.2	8
70	Step structure of Si(110)-(16Ã—2)and adsorption ofH2O. Physical Review B, 2010, 82, .	3.2	13
71	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
72	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

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73	Chemical accuracy for the van der Waals density functional. Journal of Physics Condensed Matter, 2010, 22, 022201.	1.8	2,222
74	Adsorption of Thiophene-Conjugated Sensitizers on TiO₂ Anatase (101). Journal of Physical Chemistry C, 2010, 114, 20240-20248.	3.1	40
75	Atomic-scale nanowires on Si(001): Cu on Bi. Physical Review B, 2010, 82, .	3.2	4
76	Adsorption of Catechol on TiO₂ Rutile (100): A Density Functional Theory Investigation. Journal of Physical Chemistry C, 2010, 114, 6491-6495.	3.1	39
77	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
78	Ab initiostudy of subsurface diffusion of Cu on the H-passivated Si(001) surface. Physical Review B, 2009, 80, .	3.2	8
79	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
80	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
81	Pseudo-atomic orbitals as basis sets for the O(N) DFT code CONQUEST. Journal of Physics Condensed Matter, 2008, 20, 294206.	1.8	31
82	Accuracy of order-Ndensity-functional theory calculations on DNA systems using CONQUEST. Journal of Physics Condensed Matter, 2008, 20, 294201.	1.8	25
83	Atomic structure of misfit dislocations at InAs/GaAs(110). Journal of Physics Condensed Matter, 2008, 20, 235227.	1.8	11
84	Automatic data distribution and load balancing with space-filling curves: implementation in CONQUEST. Journal of Physics Condensed Matter, 2008, 20, 275223.	1.8	10
85	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
86	Molecular interactions and decomposition pathways ofNH3on Si(001). Physical Review B, 2007, 75, .	3.2	34
87	Density functional calculations of Ge(105): Local basis sets andO(N)methods. Physical Review B, 2007, 76, .	3.2	16
88	Dynamical simulation of inelastic quantum transport. Journal of Physics Condensed Matter, 2007, 19, 196201.	1.8	61
89	Order-N first-principles calculations with the conquest code. Computer Physics Communications, 2007, 177, 14-18.	7.5	64
90	The transfer of energy between electrons and ions in solids. Reports on Progress in Physics, 2006, 69, 1195-1234.	20.1	77

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91	Molecular conduction: Do time-dependent simulations tell you more than the Landauer approach?. Journal of Chemical Physics, 2006, 124, 214708.	3.0	75
92	1D semiconducting atomic chain of In and Bi on Si(001). Journal of Physics Condensed Matter, 2006, 18, L241-L249.	1.8	7
93	Recent progress with large-scaleab initio calculations: the CONQUEST code. Physica Status Solidi (B): Basic Research, 2006, 243, 989-1000.	1.5	181
94	Self-assembled nanowires on semiconductor surfaces. Journal of Materials Science, 2006, 41, 4568-4603.	3.7	89
95	Comment on â€˜Bi nanolines on Si(001): registry with substrateâ€™. Nanotechnology, 2006, 17, 1801-1802.	2.6	4
96	Electronic state of interstitial Cu in bulk Si: Density functional calculations. Physical Review B, 2006, 73, .	3.2	11
97	Adsorption of pentacene on a silicon surface. Surface Science, 2005, 578, 20-26.	1.9	45
98	Group V dimers on Si(001): Can they act as Lewis bases?. Surface Science, 2005, 595, 233-238.	1.9	2
99	Identification of intermediate linear structure formed during Bi/Si(001) surface anneal. Surface Science, 2005, 596, 163-175.	1.9	11
100	Correlated electronâ€“ion dynamics with open boundaries: formalism. Journal of Physics Condensed Matter, 2005, 17, 3985-3995.	1.8	14
101	Encapsulation of atomic-scale Bi wires in epitaxial silicon without loss of structure. Physical Review B, 2005, 72, .	3.2	22
102	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
103	Correlated electronâ€“ion dynamics: the excitation of atomic motion by energetic electrons. Journal of Physics Condensed Matter, 2005, 17, 4793-4812.	1.8	57
104	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
105	Short range and long range strain fields of Bi nanoline. Materials Science and Technology, 2004, 20, 955-958.	1.6	4
106	Beyond Ehrenfest: correlated non-adiabatic molecular dynamics. Journal of Physics Condensed Matter, 2004, 16, 8251-8266.	1.8	86
107	Tight binding studies of strained Ge/Si() growth. Surface Science, 2003, 526, 356-366.	1.9	15
108	Interaction between electronic structure and strain in Bi nanolines on Si(001). Surface Science, 2003, 527, L177-L183.	1.9	36

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109	A first principles study of sub-monolayer Ge on Si(). Surface Science, 2002, 515, 483-490.	1.9	23
110	Parallel sparse matrix multiplication for linear scaling electronic structure calculations. Computer Physics Communications, 2001, 137, 255-273.	7.5	42
111	Small polaron formation in dangling-bond wires on the Si(001) surface. Physical Review B, 2000, 63, .	3.2	18
112	Structure of atomically perfect lines of bismuth in the Si(001) surface. Physical Review B, 2000, 62, 7237-7242.	3.2	27
113	Density matrices in O(N) electronic structure calculations: theory and applications. Computer Physics Communications, 1999, 120, 95-108.	7.5	52
114	What to do with All the Numbers. , 0, , 235-252.		0
115	Coordinates and Simulation Cell. , 0, , 165-191.		0