David Drabold

List of Publications by Year
in descending order

98 papers	5,771 citations	66234 42 h-index	76769 74 g-index
98 all docs	98 docs citations	98 times ranked	4109 citing authors

#	Article	IF	Citations
1	Unconstrained minimization approach for electronic computations that scales linearly with system size. Physical Review B, 1993, 48, 14646-14649.	1.1	377
2	Linear system-size scaling methods for electronic-structure calculations. Physical Review B, 1995, 51, 1456-1476.	1.1	253
3	Advances and applications in the F<scp>IREBALL</scp>ab initio tightâ€binding molecularâ€dynamics formalism. Physica Status Solidi (B): Basic Research, 2011, 248, 1989-2007.	0.7	207
4	Energetics of Large Fullerenes: Balls, Tubes, and Capsules. Science, 1992, 256, 1792-1795.	6.0	197
5	Maximum entropy approach for linear scaling in the electronic structure problem. Physical Review Letters, 1993, 70, 3631-3634.	2.9	197
6	Origins of structural and electronic transitions in disordered silicon. Nature, 2021, 589, 59-64.	13.7	192
7	Theory of diamondlike amorphous carbon. Physical Review B, 1994, 49, 16415-16422.	1.1	182
8	Properties of amorphous and crystalline titanium dioxide from first principles. Journal of Materials Science, 2012, 47, 7515-7521.	1.7	173
9	Molecular-dynamics determination of electronic and vibrational spectra, and equilibrium structures of small Si clusters. Physical Review B, 1990, 41, 12750-12759.	1.1	148
10	Order-Nprojection method for first-principles computations of electronic quantities and Wannier functions. Physical Review B, 1998, 57, 6391-6407.	1.1	133
11	Atomistic Structure of Band-Tail States in Amorphous Silicon. Physical Review Letters, 1998, 80, 1928-1931.	2.9	130
12	Ab initiostudy of diamond C(100) surfaces. Physical Review B, 1993, 48, 5261-5264.	1.1	120
13	Abinitiomolecular-dynamics study of the structural, vibrational, and electronic properties of glassyGeSe2. Physical Review B, 1996, 54, 12162-12171.	1.1	120
14	Structure and energetics of giant fullerenes: An order-Nmolecular-dynamics study. Physical Review B, 1996, 53, 2132-2140.	1.1	115
15	Topics in the theory of amorphous materials. European Physical Journal B, 2009, 68, 1-21.	0.6	114
16	Atomistic Origin of Urbach Tails in Amorphous Silicon. Physical Review Letters, 2008, 100, 206403.	2.9	106
17	Finite-temperature properties of amorphous silicon. Physical Review Letters, 1991, 67, 2179-2182.	2.9	100
18	Can Amorphous GaN Serve as a Useful Electronic Material?. Physical Review Letters, 1997, 79, 677-680.	2.9	100

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19	Linear Scaling Method for Phonon Calculations from Electronic Structure. Physical Review Letters, 1995, 75, 1324-1327.	2.9	98
20	Structure Determination of Disordered Materials from Diffraction Data. Physical Review Letters, 2010, 104, 125501.	2.9	97
21	Kernel polynomial method for a nonorthogonal electronic-structure calculation of amorphous diamond. Physical Review B, 1997, 55, 15382-15385.	1.1	95
22	Direct Molecular Dynamic Simulation of Light-Induced Structural Change in Amorphous Selenium. Physical Review Letters, 1999, 83, 5042-5045.	2.9	92
23	Density functional studies of small platinum clusters. Journal of Physics Condensed Matter, 1997, 9, L39-L45.	0.7	89
24	Molecular-dynamics simulations of amorphous Si. Physical Review B, 1990, 42, 5135-5141.	1.1	88
25	First-principles local-orbital density-functional study of Al clusters. Physical Review B, 1993, 47, 1567-1576.	1.1	87
26	Direct Calculation of Light-Induced Structural Change and Diffusive Motion in GlassyAs2Se3. Physical Review Letters, 2000, 85, 2785-2788.	2.9	86
27	Structure and physical properties of paracrystalline atomistic models of amorphous silicon. Journal of Applied Physics, 2001, 90, 4437-4451.	1.1	85
28	Structural, electronic, and vibrational properties of diamond (100), (111), and (110) surfaces fromab initiocalculations. Physical Review B, 1995, 51, 14669-14685.	1.1	70
29	Ab initiomolecular-dynamics study of liquidGeSe2. Physical Review B, 1997, 56, 3054-3065.	1.1	69
30	Defects, doping, and conduction mechanisms in nitrogen-doped tetrahedral amorphous carbon. Journal of Applied Physics, 1997, 81, 1289-1295.	1.1	67
31	Phonon modes of diamond (100) surfaces fromab initiocalculations. Physical Review B, 1995, 51, 1989-1992.	1.1	63
32	Atomistic origins of light-induced defects ina-Si. Physical Review Letters, 1992, 68, 1888-1891.	2.9	61
33	Defects, tight binding, and first-principles molecular-dynamics simulations ona-Si. Physical Review B, 1992, 45, 4048-4055.	1.1	61
34	Band gap engineering in amorphous AlxGa1â^'xN: Experiment andab initiocalculations. Applied Physics Letters, 2000, 77, 1117-1119.	1.5	59
35	Observation of light polarization-dependent structural changes in chalcogenide glasses. Applied Physics Letters, 2003, 82, 706-708.	1.5	55
36	Electronic structure of schwarzite. Physical Review B, 1992, 46, 1941-1943.	1.1	54

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37	Theoretical study on the nature of band-tail states in amorphous Si. Physical Review B, 1998, 58, 15624-15631.	1.1	50
38	Evolution of amorphous carbon across densities: An inferential study. Carbon, 2018, 131, 168-174.	5.4	49
39	Neutron-scattering andab initiomolecular-dynamics study of vibrations in glassyGeSe2. Physical Review B, 1995, 52, 9133-9136.	1.1	48
40	Gap formation and defect states in tetrahedral amorphous carbon. Physical Review B, 1996, 54, 5480-5484.	1.1	48
41	Structural and electronic properties of glassyGeSe2surfaces. Physical Review B, 2000, 62, 15695-15701.	1.1	45
42	Projected random vectors and the recursion method in the electronic-structure problem. Physical Review B, 1994, 50, 1376-1381.	1.1	44
43	Exciton-induced lattice relaxation and the electronic and vibrational spectra of silicon clusters. Physical Review B, 1996, 53, 8042-8051.	1.1	42
44	Hydrogen and defects in first-principles molecular-dynamics-modeleda-Si:H. Physical Review B, 1993, 47, 13277-13282.	1.1	41
45	Atomic layering at the liquid silicon surface: A first-principles simulation. Physical Review B, 1999, 60, R16283-R16286.	1.1	39
46	Study of structural changes in amorphous As2Se3 by EXAFS under in situ laser irradiation. Solid State Communications, 2001, 120, 149-153.	0.9	39
47	Universal features of localized eigenstates in disordered systems. Journal of Physics Condensed Matter, 2005, 17, L321-L327.	0.7	38
48	Ab initioestimate of temperature dependence of electrical conductivity in a model amorphous material: Hydrogenated amorphous silicon. Physical Review B, 2007, 76, .	1.1	38
49	Efficientab initiomolecular-dynamics simulations of carbon. Physical Review B, 1991, 43, 5132-5134.	1.1	36
50	Band-tail states and the localized-to-extended transition in amorphous diamond. Physical Review B, 1996, 54, 10284-10287.	1.1	35
51	Quantifying Chemical Structure and Machineâ€Learned Atomic Energies in Amorphous and Liquid Silicon. Angewandte Chemie - International Edition, 2019, 58, 7057-7061.	7.2	35
52	First-principles molecular-dynamics study of glassyAs2Se3. Physical Review B, 2000, 61, 11998-12004.	1.1	34
53	Physical, structural, and shielding properties of cadmium bismuth borate-based glasses. Journal of Applied Physics, 2020, 127, .	1.1	34
54	Ring formation and the structural and electronic properties of tetrahedral amorphous carbon surfaces. Physical Review B, 1998, 57, 15591-15598.	1.1	32

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55	Pentagonal puckering in a sheet of amorphous graphene. Physica Status Solidi (B): Basic Research, 2011, 248, 2082-2086.	0.7	31
56	Amorphous carbon at low densities: An ab initio study. Carbon, 2017, 115, 532-538.	5.4	30
57	Convergence of force calculations for noncrystalline Si. Physical Review B, 1990, 42, 5345-5348.	1.1	29
58	Electrical conductivity and Meyerâ€“Neldel rule: The role of localized states in hydrogenated amorphous silicon. Journal of Non-Crystalline Solids, 2008, 354, 2909-2913.	1.5	29
59	Low-temperature anomalous specific heat without tunneling modes: A simulation foraâ^'Siwith voids. Physical Review B, 2000, 61, 5376-5380.	1.1	28
60	Approximateab initiocalculations of electronic structure of amorphous silicon. Physical Review B, 2000, 62, 15307-15310.	1.1	26
61	Spatial Decay of the Single-Particle Density Matrix in Insulators: Analytic Results in Two and Three Dimensions. Physical Review Letters, 2002, 88, 196405.	2.9	25
62	Amorphous graphene: a constituent part of low density amorphous carbon. Physical Chemistry Chemical Physics, 2018, 20, 19546-19551.	1.3	25
63	AbÂInitio Simulation of Amorphous Graphite. Physical Review Letters, 2022, 128, .	2.9	25
64	Ab initiostudies of hydrocarbon adsorption on stepped diamond surfaces. Physical Review B, 1994, 50, 15369-15380.	1.1	24
65	Density dependence of the structural and electronic properties of amorphous GaN. Solid State Communications, 1998, 108, 413-417.	0.9	24
66	Photoinduced changes in the electronic structure of As4Se3 glass. Journal of Non-Crystalline Solids, 2004, 349, 162-167.	1.5	24
67	Electronic consequences of the mutual presence of thermal and structural disorder. Physical Review B, 1999, 60, R721-R725.	1.1	23
68	Real space information from fluctuation electron microscopy: applications to amorphous silicon. Journal of Physics Condensed Matter, 2007, 19, 455202.	0.7	23
69	Vibrations in amorphous silica. Journal of Non-Crystalline Solids, 2016, 439, 6-14.	1.5	23
70	An intermediate phase in GexSe1â^'xglasses: experiment and simulation. Journal of Physics Condensed Matter, 2007, 19, 455206.	0.7	22
71	Large and realistic models of amorphous silicon. Journal of Non-Crystalline Solids, 2018, 492, 27-32.	1.5	22
72	Molecular-dynamics investigations of conformational fluctuations and low-energy vibrational excitations ina-Si:H. Physical Review B, 1996, 53, 3841-3845.	1.1	20

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73	Theory of boron doping ina-Si:H. Physical Review B, 1997, 56, 1864-1867.	1.1	20
74	Topological and topological-electronic correlations in amorphous silicon. Journal of Non-Crystalline Solids, 2008, 354, 3480-3485.	1.5	18
75	Competing stoichiometric phases and the intermediate phase in Ge_xSe_{1â^'x} glasses. Physica Status Solidi (B): Basic Research, 2009, 246, 1849-1853.	0.7	18
76	Hidden structure in amorphous solids. Physica Status Solidi (A) Applications and Materials Science, 2010, 207, 599-604.	0.8	18
77	Symmetry breaking and low energy conformational fluctuations in amorphous graphene. Physica Status Solidi (B): Basic Research, 2013, 250, 1012-1019.	0.7	18
78	Quantifying Chemical Structure and Machineâ€Learned Atomic Energies in Amorphous and Liquid Silicon. Angewandte Chemie, 2019, 131, 7131-7135.	1.6	18
79	Ab initiosimulation of solid electrolyte materials in liquid and glassy phases. Physical Review B, 2011, 83, .	1.1	17
80	Approximate ab initio simulations of amorphous silicon and glassy chalcogenides. Current Opinion in Solid State and Materials Science, 2001, 5, 509-516.	5.6	13
81	Network structure and dynamics of hydrogenated amorphous silicon. Journal of Non-Crystalline Solids, 2008, 354, 2149-2154.	1.5	12
82	Phonon driven transport in amorphous semiconductors: transition probabilities. European Physical Journal B, 2010, 77, 7-23.	0.6	12
83	Structural origins of electronic conduction in amorphous copper-doped alumina. Physical Review Materials, 2019, 3, .	0.9	12
84	Electronically designed amorphous carbon and silicon. Physica Status Solidi (A) Applications and Materials Science, 2016, 213, 1653-1660.	0.8	10
85	Spatial Projection of Electronic Conductivity: The Example of Conducting Bridge Memory Materials. Physica Status Solidi - Rapid Research Letters, 2018, 12, 1800238.	1.2	10
86	Directab initio simulation of silver ion dynamics in chalcogenide glasses. Physica Status Solidi (B): Basic Research, 2005, 242, R55-R57.	0.7	9
87	Silicon: the gulf between crystalline and amorphous. Physica Status Solidi - Rapid Research Letters, 2011, 5, 359-360.	1.2	7
88	Structure and charge transport of amorphous Cu-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ta</mml:mi><mml:mn>2</mml:mn></mml:r mathvariant="normal">O</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:mrow></mml:math> : An ab initio study. Physical Review Materials, 2020, 4, .	0.9	7
89	Ab initio inversion of structure and the lattice dynamics of a metallic glass: the case of Pd₄₀Ni₄₀P₂₀. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 075002.	0.8	5
90	Electrical conduction processes in aluminum: Defects and phonons. Physical Review B, 2022, 105, .	1.1	5

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91	Semiquantitative scattering theory of amorphous materials. Physical Review B, 2008, 78, .	1.1	4
92	The microscopic response method: Theory of transport for systems with both topological and thermal disorder. Physica Status Solidi (B): Basic Research, 2011, 248, 2015-2026.	0.7	4
93	Electronic signatures of topological disorder in amorphous graphene. IET Circuits, Devices and Systems, 2015, 9, 13-18.	0.9	3
94	Atomic properties of sodium silicate glasses obtained from the building-block method. Physical Review B, 2021, 103, .	1.1	3
95	Realistic computer models of amorphous <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZrO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> : <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ta</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>5</mml:mn></mml:mrow></mml:math> : Structural, optical, and vibrational properties. Physical Review B, 2022, 105, .	1.1	3
96	Atomistic Simulation of the Finite-Temperature Anderson Localization Problem. Physica Status Solidi (B): Basic Research, 2002, 233, 10-17.	0.7	2
97	Symmetry breaking and low energy conformational fluctuations in amorphous graphene. Physica Status Solidi (B): Basic Research, 2013, 250, 1011-1011.	0.7	2
98	Radiation fields for nanoscale systems. Physica Status Solidi (B): Basic Research, 2013, 250, 1052-1061.	0.7	1