David Drabold

List of Publications by Citations

94 papers	4,957 citations	40 h-index	68 g-index
98 ext. papers	5,298 ext. citations	4.5 avg, IF	5.49 L-index

#	Paper	IF	Citations
94	Unconstrained minimization approach for electronic computations that scales linearly with system size. *Physical Review B*, **1993**, 48, 14646-14649	3.3	325
93	Linear system-size scaling methods for electronic-structure calculations. *Physical Review B*, **1995**, 51, 1456-1476	3.3	231
92	Energetics of large fullerenes: balls, tubes, and capsules. *Science*, **1992**, 256, 1792-5	33.3	188
91	Theory of diamondlike amorphous carbon. *Physical Review B*, **1994**, 49, 16415-16422	3.3	173
90	Advances and applications in the FIREBALL ab initio tight-binding molecular-dynamics formalism. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 1989-2007	1.3	169
89	Maximum entropy approach for linear scaling in the electronic structure problem. *Physical Review Letters*, **1993**, 70, 3631-3634	7.4	160
88	Properties of amorphous and crystalline titanium dioxide from first principles. *Journal of Materials Science*, **2012**, 47, 7515-7521	4.3	146
87	Molecular-dynamics determination of electronic and vibrational spectra, and equilibrium structures of small Si clusters. *Physical Review B*, **1990**, 41, 12750-12759	3.3	142
86	Atomistic Structure of Band-Tail States in Amorphous Silicon. *Physical Review Letters*, **1998**, 80, 1928-1931	7.4	124
85	Ab initio molecular-dynamics study of the structural, vibrational, and electronic properties of glassy GeSe2. *Physical Review B*, **1996**, 54, 12162-12171	3.3	114
84	Ab initio study of diamond C(100) surfaces. *Physical Review B*, **1993**, 48, 5261-5264	3.3	112
83	Order-N projection method for first-principles computations of electronic quantities and Wannier functions. *Physical Review B*, **1998**, 57, 6391-6407	3.3	107
82	Topics in the theory of amorphous materials. *European Physical Journal B*, **2009**, 68, 1-21	1.2	96
81	Atomistic origin of urbach tails in amorphous silicon. *Physical Review Letters*, **2008**, 100, 206403	7.4	95
80	Can Amorphous GaN Serve as a Useful Electronic Material?. *Physical Review Letters*, **1997**, 79, 677-680	7.4	94
79	Finite-temperature properties of amorphous silicon. *Physical Review Letters*, **1991**, 67, 2179-2182	7.4	92
78	Structure determination of disordered materials from diffraction data. *Physical Review Letters*, **2010**, 104, 125501	7.4	88

77	Structure and energetics of giant fullerenes: An order-N molecular-dynamics study. *Physical Review B*, **1996**, 53, 2132-2140	3.3	86
76	Molecular-dynamics simulations of amorphous Si. *Physical Review B*, **1990**, 42, 5135-5141	3.3	86
75	Direct Molecular Dynamic Simulation of Light-Induced Structural Change in Amorphous Selenium. *Physical Review Letters*, **1999**, 83, 5042-5045	7.4	84
74	First-principles local-orbital density-functional study of Al clusters. *Physical Review B*, **1993**, 47, 1567-1576	3.3	82
73	Density functional studies of small platinum clusters. *Journal of Physics Condensed Matter*, **1997**, 9, L39-L48	1.8	81
72	Direct calculation of light-induced structural change and diffusive motion in glassy As2Se3. *Physical Review Letters*, **2000**, 85, 2785-8	7.4	77
71	Structure and physical properties of paracrystalline atomistic models of amorphous silicon. *Journal of Applied Physics*, **2001**, 90, 4437-4451	2.5	75
70	Linear scaling method for phonon calculations from electronic structure. *Physical Review Letters*, **1995**, 75, 1324-1327	7.4	73
69	Kernel polynomial method for a nonorthogonal electronic-structure calculation of amorphous diamond. *Physical Review B*, **1997**, 55, 15382-15385	3.3	70
68	Ab initio molecular-dynamics study of liquid GeSe2. *Physical Review B*, **1997**, 56, 3054-3065	3.3	69
67	Structural, electronic, and vibrational properties of diamond (100), (111), and (110) surfaces from ab initio calculations. *Physical Review B*, **1995**, 51, 14669-14685	3.3	66
66	Origins of structural and electronic transitions in disordered silicon. *Nature*, **2021**, 589, 59-64	50.4	66
65	Phonon modes of diamond (100) surfaces from ab initio calculations. *Physical Review B*, **1995**, 51, 1989-1992	3.3	63
64	Defects, doping, and conduction mechanisms in nitrogen-doped tetrahedral amorphous carbon. *Journal of Applied Physics*, **1997**, 81, 1289-1295	2.5	61
63	Defects, tight binding, and first-principles molecular-dynamics simulations on a-Si. *Physical Review B* , **1992**, 45, 4048-4055	3.3	60
62	Atomistic origins of light-induced defects in a-Si. *Physical Review Letters*, **1992**, 68, 1888-1891	7.4	58
61	Band gap engineering in amorphous AlxGa1−xN: Experiment and ab initio calculations. *Applied Physics Letters*, **2000**, 77, 1117-1119	3.4	55
60	Theoretical study on the nature of band-tail states in amorphous Si. *Physical Review B*, **1998**, 58, 15624-15631	3.3	46

59	Neutron-scattering and ab initio molecular-dynamics study of vibrations in glassy GeSe2. *Physical Review B*, **1995**, 52, 9133-9136	3.3	46
58	Gap formation and defect states in tetrahedral amorphous carbon. *Physical Review B*, **1996**, 54, 5480-5484	3.3	45
57	Electronic structure of schwarzite. *Physical Review B*, **1992**, 46, 1941-1943	3.3	43
56	Structural and electronic properties of glassy GeSe2 surfaces. *Physical Review B*, **2000**, 62, 15695-15701	3.3	40
55	Projected random vectors and the recursion method in the electronic-structure problem. *Physical Review B*, **1994**, 50, 1376-1381	3.3	40
54	Exciton-induced lattice relaxation and the electronic and vibrational spectra of silicon clusters. *Physical Review B*, **1996**, 53, 8042-8051	3.3	39
53	Hydrogen and defects in first-principles molecular-dynamics-modeled a-Si:H. *Physical Review B*, **1993**, 47, 13277-13282	3.3	39
52	Observation of light polarization-dependent structural changes in chalcogenide glasses. *Applied Physics Letters*, **2003**, 82, 706-708	3.4	38
51	Atomic layering at the liquid silicon surface: A first-principles simulation. *Physical Review B*, **1999**, 60, R16283-R16286	3.3	37
50	Study of structural changes in amorphous As2Se3 by EXAFS under in situ laser irradiation. *Solid State Communications*, **2001**, 120, 149-153	1.6	36
49	Universal features of localized eigenstates in disordered systems. *Journal of Physics Condensed Matter*, **2005**, 17, L321-L327	1.8	34
48	Ab initio estimate of temperature dependence of electrical conductivity in a model amorphous material: Hydrogenated amorphous silicon. *Physical Review B*, **2007**, 76,	3.3	33
47	Efficient ab initio molecular-dynamics simulations of carbon. *Physical Review B*, **1991**, 43, 5132-5134	3.3	33
46	Ring formation and the structural and electronic properties of tetrahedral amorphous carbon surfaces. *Physical Review B*, **1998**, 57, 15591-15598	3.3	31
45	First-principles molecular-dynamics study of glassy As2Se3. *Physical Review B*, **2000**, 61, 11998-12004	3.3	29
44	Low-temperature anomalous specific heat without tunneling modes: A simulation for a-Si with voids. *Physical Review B*, **2000**, 61, 5376-5380	3.3	28
43	Band-tail states and the localized-to-extended transition in amorphous diamond. *Physical Review B*, **1996**, 54, 10284-10287	3.3	28
42	Evolution of amorphous carbon across densities: An inferential study. *Carbon*, **2018**, 131, 168-174	10.4	27

41	Electrical conductivity and Meyer-Neldel rule: The role of localized states in hydrogenated amorphous silicon. *Journal of Non-Crystalline Solids*, **2008**, 354, 2909-2913	3.9	27
40	Quantifying Chemical Structure and Machine-Learned Atomic Energies in Amorphous and Liquid Silicon. *Angewandte Chemie - International Edition*, **2019**, 58, 7057-7061	16.4	26
39	Approximate ab initio calculations of electronic structure of amorphous silicon. *Physical Review B*, **2000**, 62, 15307-15310	3.3	26
38	Convergence of force calculations for noncrystalline Si. *Physical Review B*, **1990**, 42, 5345-5348	3.3	26
37	Spatial decay of the single-particle density matrix in insulators: analytic results in two and three dimensions. *Physical Review Letters*, **2002**, 88, 196405	7.4	25
36	Pentagonal puckering in a sheet of amorphous graphene. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 2082-2086	1.3	23
35	Real space information from fluctuation electron microscopy: applications to amorphous silicon. *Journal of Physics Condensed Matter*, **2007**, 19, 455202	1.8	23
34	Ab initio studies of hydrocarbon adsorption on stepped diamond surfaces. *Physical Review B*, **1994**, 50, 15369-15380	3.3	23
33	Density dependence of the structural and electronic properties of amorphous GaN. *Solid State Communications*, **1998**, 108, 413-417	1.6	22
32	Photoinduced changes in the electronic structure of As4Se3 glass. *Journal of Non-Crystalline Solids*, **2004**, 349, 162-167	3.9	22
31	Electronic consequences of the mutual presence of thermal and structural disorder. *Physical Review B*, **1999**, 60, R721-R725	3.3	22
30	An intermediate phase in GexSe1−xglasses: experiment and simulation. *Journal of Physics Condensed Matter*, **2007**, 19, 455206	1.8	20
29	Molecular-dynamics investigations of conformational fluctuations and low-energy vibrational excitations in a-Si:H. *Physical Review B*, **1996**, 53, 3841-3845	3.3	20
28	Amorphous carbon at low densities: An ab initio study. *Carbon*, **2017**, 115, 532-538	10.4	19
27	Physical, structural, and shielding properties of cadmium bismuth borate-based glasses. *Journal of Applied Physics*, **2020**, 127, 175102	2.5	19
26	Large and realistic models of amorphous silicon. *Journal of Non-Crystalline Solids*, **2018**, 492, 27-32	3.9	18
25	Competing stoichiometric phases and the intermediate phase in GexSe1−x glasses. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 1849-1853	1.3	18
24	Amorphous graphene: a constituent part of low density amorphous carbon. *Physical Chemistry Chemical Physics*, **2018**, 20, 19546-19551	3.6	17

23	Topological and topological-electronic correlations in amorphous silicon. *Journal of Non-Crystalline Solids*, **2008**, 354, 3480-3485	3.9	17
22	Theory of boron doping in a-Si:H. *Physical Review B*, **1997**, 56, 1864-1867	3.3	16
21	Vibrations in amorphous silica. *Journal of Non-Crystalline Solids*, **2016**, 439, 6-14	3.9	15
20	Symmetry breaking and low energy conformational fluctuations in amorphous graphene. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 1012-1019	1.3	15
19	Hidden structure in amorphous solids. *Physica Status Solidi (A) Applications and Materials Science*, **2010**, 207, 599-604	1.6	15
18	Ab initio simulation of solid electrolyte materials in liquid and glassy phases. *Physical Review B*, **2011**, 83,	3.3	14
17	Quantifying Chemical Structure and Machine-Learned Atomic Energies in Amorphous and Liquid Silicon. *Angewandte Chemie*, **2019**, 131, 7131-7135	3.6	12
16	Network structure and dynamics of hydrogenated amorphous silicon. *Journal of Non-Crystalline Solids*, **2008**, 354, 2149-2154	3.9	12
15	Approximate ab initio simulations of amorphous silicon and glassy chalcogenides. *Current Opinion in Solid State and Materials Science*, **2001**, 5, 509-516	12	12
14	Phonon driven transport in amorphous semiconductors: transition probabilities. *European Physical Journal B*, **2010**, 77, 7-23	1.2	11
13	Direct ab initio simulation of silver ion dynamics in chalcogenide glasses. *Physica Status Solidi (B): Basic Research*, **2005**, 242, R55-R57	1.3	8
12	Electronically designed amorphous carbon and silicon. *Physica Status Solidi (A) Applications and Materials Science*, **2016**, 213, 1653-1660	1.6	7
11	Silicon: the gulf between crystalline and amorphous. *Physica Status Solidi - Rapid Research Letters*, **2011**, 5, 359-360	2.5	7
10	Structural origins of electronic conduction in amorphous copper-doped alumina. *Physical Review Materials*, **2019**, 3,	3.2	7
9	Spatial Projection of Electronic Conductivity: The Example of Conducting Bridge Memory Materials. *Physica Status Solidi - Rapid Research Letters*, **2018**, 12, 1800238	2.5	6
8	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	1.3	4
7	Semiquantitative scattering theory of amorphous materials. *Physical Review B*, **2008**, 78,	3.3	4
6	Structure and charge transport of amorphous Cu-doped Ta2O5: An ab initio study. *Physical Review Materials*, **2020**, 4,	3.2	4

5	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	2	3
4	Electronic signatures of topological disorder in amorphous graphene. *IET Circuits, Devices and Systems*, **2015**, 9, 13-18	1.1	3
3	Symmetry breaking and low energy conformational fluctuations in amorphous graphene. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 1011-1011	1.3	2
2	Atomistic Simulation of the Finite-Temperature Anderson Localization Problem. *Physica Status Solidi (B): Basic Research*, **2002**, 233, 10-17	1.3	2
1	Radiation fields for nanoscale systems. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 1052-1061	1.3	1