D W Brenner

List of Publications by Year
in descending order

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59 papers	4,316 citations	257450 24 h-index	214800 47 g-index
60 all docs	60 docs citations	60 times ranked	3837 citing authors

#	Article	IF	Citations
1	Energetics of nanoscale graphitic tubules. Physical Review B, 1992, 45, 12592-12595.	3.2	893
2	Carbon Nanostructures. Critical Reviews in Solid State and Materials Sciences, 2002, 27, 227-356.	12.3	708
3	Molecular Simulation of the Influence of Chemical Cross-Links on the Shear Strength of Carbon Nanotubeâ˜Polymer Interfaces. Journal of Physical Chemistry B, 2002, 106, 3046-3048.	2.6	585
4	Atomistic modeling of the fracture of polycrystalline diamond. Physical Review B, 2000, 61, 3877-3888.	3.2	362
5	Molecular-dynamics simulations of atomic-scale friction of diamond surfaces. Physical Review B, 1992, 46, 9700-9708.	3.2	250
6	Molecular Dynamics Simulations of Dimer Opening on a Diamond Â(2x1) Surface. Science, 1992, 255, 835-838.	12.6	201
7	Simulations of buckminsterfullerene (C60) collisions with a hydrogen-terminated diamond {111} surface. The Journal of Physical Chemistry, 1991, 95, 7138-7142.	2.9	144
8	Detonations at nanometer resolution using molecular dynamics. Physical Review Letters, 1993, 70, 2174-2177.	7.8	137
9	Charge compensation and electrostatic transferability in three entropy-stabilized oxides: Results from density functional theory calculations. Journal of Applied Physics, 2016, 120, .	2.5	100
10	Local density functional electronic structures of three stable icosahedral fullerenes. The Journal of Physical Chemistry, 1991, 95, 8737-8741.	2.9	92
11	Anisotropic spread of surface dimer openings in the initial stages of the epitaxial growth of Si on Si{100}. Physical Review Letters, 1989, 63, 302-305.	7.8	73
12	Ion pickup of large, surface-adsorbed molecules: a demonstration of the Eley-Rideal mechanism. Journal of the American Chemical Society, 1992, 114, 3207-3210.	13.7	70
13	Predicted structure and electronic properties of individual carbon nanocones and nanostructures assembled from nanocones. Nanotechnology, 2001, 12, 191-197.	2.6	61
14	Split shock waves from molecular dynamics. Physical Review Letters, 1991, 67, 3132-3135.	7.8	57
15	Local-density-functional calculation of photoelectron spectra of fullerenes. Physical Review B, 1991, 43, 14281-14284.	3.2	56
16	Influence of mass and charge disorder on the phonon thermal conductivity of entropy stabilized oxides determined by molecular dynamics simulations. Journal of Applied Physics, 2019, 125, .	2.5	48
17	Free energies of (Co, Fe, Ni, Zn)Fe₂O₄spinels and oxides in water at high temperatures and pressure from density functional theory: results for stoichiometric NiO and NiFe₂O₄surfaces. Journal of Physics Condensed Matter, 2013, 25, 445008.	1.8	47
18	Multiscale modeling approach for calculating grain-boundary energies from first principles. Physical Review B, 1998, 57, R3181-R3184.	3.2	46

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19	The adsorption of aflatoxin B1 by detonation-synthesis nanodiamonds. Doklady Biochemistry and Biophysics, 2007, 417, 299-301.	0.9	46
20	Molecular Dynamics Simulations of Carbon Nanotube Rolling and Sliding on Graphite. Molecular Simulation, 2000, 25, 73-79.	2.0	43
21	Immobilization of mycotoxins on modified nanodiamond substrates. Biointerphases, 2011, 6, 210-217.	1.6	41
22	Atomistic simulations of structures and mechanical properties of polycrystalline diamond: Symmetrical ã€ˆ001ã€‰ tilt grain boundaries. Physical Review B, 1999, 60, 7043-7052.	3.2	38
23	The role of creep in the time-dependent resistance of Ohmic gold contacts in radio frequency microelectromechanical system devices. Journal of Applied Physics, 2008, 104, .	2.5	28
24	Group-IV covalent clusters:Si45andC44versusSi44andC45. Physical Review B, 1991, 44, 3479-3482.	3.2	26
25	Elastic models of symmetrical ã€ˆ001ã€‰ and ã€ˆ011ã€‰ tilt grain boundaries in diamond. Physical Review B, 2000, 61, 928-936.	3.2	21
26	Atomistic Simulation of the Nanoindentation of Diamond and Graphite Surfaces. Materials Research Society Symposia Proceedings, 1991, 239, 573.	0.1	17
27	Fullerene/Tubule Based Hollow Carbon Nano-Gears. Materials Research Society Symposia Proceedings, 1994, 349, 283.	0.1	16
28	Exchange interactions and long-range magnetic order in the (Mg,Co,Cu,Ni,Zn)O entropy-stabilized oxide: A theoretical investigation. Journal of Applied Physics, 2020, 127, .	2.5	16
29	Reinforcement Mechanisms in Polymer Nanotube Composites: Simulated Non-Bonded and Cross-Linked Systems. Materials Research Society Symposia Proceedings, 2000, 633, 14171.	0.1	11
30	Molecular Dynamics Simulations of Polymer-Nanotube Composites. Materials Research Society Symposia Proceedings, 1999, 593, 199.	0.1	10
31	Nanoindentation as a Probe of Nanoscale Residual Stresses: Atomistic Simulation Results. Molecular Simulation, 2000, 25, 81-91.	2.0	10
32	First-principles investigation of diffusion and defect properties of Fe and Ni in Cr2O3. Journal of Applied Physics, 2018, 123, .	2.5	10
33	Chemistry and phase transitions from hypervelocity impacts. International Journal of Quantum Chemistry, 1994, 52, 129-137.	2.0	8
34	Coexistence Of Two Carbon Phases At Grain Boundaries In Polycrystalline Diamond. Materials Research Society Symposia Proceedings, 1996, 442, 693.	0.1	4
35	Hierarchical modeling of nanoindentation and microstructural evolution of face-centered cubic gold aggregates. Journal of Materials Research, 2007, 22, 627-643.	2.6	4
36	Negative Surface Energies of Nickel Ferrite Nanoparticles under Hydrothermal Conditions. Journal of Nanomaterials, 2019, 2019, 1-6.	2.7	4

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37	Possidle Isomers and Electronic Structure of C60H36. Materials Research Society Symposia Proceedings, 1990, 206, 687.	0.1	3
38	Ion Beam Damage of Polymer Surfaces: Insights from Molecular-Dynamics Simulation. Materials Research Society Symposia Proceedings, 1996, 438, 491.	0.1	3
39	An Evaluation of Atomic Force Microscopy as a Probe of Nanoscale Residual Stress Via Atomistic Simulation. Materials Research Society Symposia Proceedings, 1998, 522, 233.	0.1	3
40	Properties of Polycrystalline Diamond: Multiscale Modeling Approach. Molecular Simulation, 2000, 24, 197-207.	2.0	3
41	The Art and Science of an Analytic Potential. , 2005, , 23-40.		3
42	Understanding the Atomic-Level Chemistry and Structure of Oxide Deposits on Fuel Rods in Light Water Nuclear Reactors Using First Principles Methods. Jom, 2016, 68, 2912-2921.	1.9	3
43	Limits of chemical effects on cold fusion. Journal of Fusion Energy, 1990, 9, 363-366.	1.2	2
44	Linear combination of Gaussian-type orbitalsâ€“local-density-functional cluster studies of D-D interactions in titanium and palladium. Physical Review B, 1990, 41, 9683-9687.	3.2	2
45	How predictable is plastic damage at the atomic scale?. Applied Physics Letters, 2017, 110, .	3.3	2
46	Relative Energetics of C44 Fullerene Isomers. , 1992, , 1347-1351.		2
47	Dissociative Phase Transitions, Split Shock Waves, Rarefaction Shocks, and Detonations. Materials Research Society Symposia Proceedings, 1992, 296, 123.	0.1	1
48	Special C44 Isomers. Materials Research Society Symposia Proceedings, 1994, 349, 331.	0.1	1
49	Atomistic Modeling of Grain Boundary Fracture in Diamond. Materials Research Society Symposia Proceedings, 1998, 539, 319.	0.1	1
50	First-principles investigation of boron incorporation into CRUD under Pressurized Water Reactor conditions. Materials Research Society Symposia Proceedings, 2014, 1709, 1.	0.1	1
51	First-Principles Study of Photoexcited Defects in Polysilane Chains. Materials Research Society Symposia Proceedings, 1990, 209, 189.	0.1	0
52	Photoelectron Spectra of C60H36 and C60H60. Materials Research Society Symposia Proceedings, 1992, 247, 351.	0.1	0
53	Effects of crystal orientation on the properties of a chemically sustained shock wave in a model energetic material. AIP Conference Proceedings, 1994, , .	0.4	0
54	Molecular Dynamics Simulations of Hypervelocity Buckminsterfullerene Collisions. Materials Research Society Symposia Proceedings, 1994, 359, 199.	0.1	0

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55	Molecular dynamics of void collapse mechanisms in shocked media. AIP Conference Proceedings, 1994, , .	0.4	0
56	Simulations of Ozone Detonation Using a Reactive Empirical Bond Order (REBO) Potential for the Oxygen System. Materials Research Society Symposia Proceedings, 1995, 418, 301.	0.1	0
57	Detonation of solid O[sub 3]: Effects of void collapse. AIP Conference Proceedings, 1996, , .	0.4	0
58	Prediction of Energies of <100> Tilt Boundaries in Al-Pb Alloy. Materials Research Society Symposia Proceedings, 2007, 1056, 1.	0.1	0
59	Molecular Dynamics Simulation of Atomic-Scale Adhesion, Deformation, Friction, and Modification of Diamond Surfaces. , 1995, , 175-181.		0