D W Brenner

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/10400175/publications.pdf

Version: 2024-02-01

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	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
2	Negative Surface Energies of Nickel Ferrite Nanoparticles under Hydrothermal Conditions. Journal of Nanomaterials, 2019, 2019, 1-6.	2.7	4
3	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
4	First-principles investigation of diffusion and defect properties of Fe and Ni in Cr2O3. Journal of Applied Physics, 2018, 123, .	2.5	10
5	How predictable is plastic damage at the atomic scale?. Applied Physics Letters, 2017, 110, .	3.3	2
6	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
7	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
8	First-principles investigation of boron incorporation into CRUD under Pressurized Water Reactor conditions. Materials Research Society Symposia Proceedings, 2014, 1709, 1.	0.1	1
9	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
10	Immobilization of mycotoxins on modified nanodiamond substrates. Biointerphases, 2011, 6, 210-217.	1.6	41
11	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
12	Prediction of Energies of <100> Tilt Boundaries in Al-Pb Alloy. Materials Research Society Symposia Proceedings, 2007, 1056, 1.	0.1	0
13	Hierarchical modeling of nanoindentation and microstructural evolution of face-centered cubic gold aggregates. Journal of Materials Research, 2007, 22, 627-643.	2.6	4
14	The adsorption of aflatoxin B1 by detonation-synthesis nanodiamonds. Doklady Biochemistry and Biophysics, 2007, 417, 299-301.	0.9	46
15	The Art and Science of an Analytic Potential. , 2005, , 23-40.		3
16	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
17	Carbon Nanostructures. Critical Reviews in Solid State and Materials Sciences, 2002, 27, 227-356.	12.3	708
18	Predicted structure and electronic properties of individual carbon nanocones and nanostructures assembled from nanocones. Nanotechnology, 2001, 12, 191-197.	2.6	61

#	Article	IF	Citations
19	Reinforcement Mechanisms in Polymer Nanotube Composites: Simulated Non-Bonded and Cross-Linked Systems. Materials Research Society Symposia Proceedings, 2000, 633, 14171.	0.1	11
20	Elastic models of symmetrical ã€˜001ã€‰ and ã€˜011ã€‰ tilt grain boundaries in diamond. Physical Review B, 2000, 61, 928-936.	3.2	21
21	Molecular Dynamics Simulations of Carbon Nanotube Rolling and Sliding on Graphite. Molecular Simulation, 2000, 25, 73-79.	2.0	43
22	Nanoindentation as a Probe of Nanoscale Residual Stresses: Atomistic Simulation Results. Molecular Simulation, 2000, 25, 81-91.	2.0	10
23	Properties of Polycrystalline Diamond: Multiscale Modeling Approach. Molecular Simulation, 2000, 24, 197-207.	2.0	3
24	Atomistic modeling of the fracture of polycrystalline diamond. Physical Review B, 2000, 61, 3877-3888.	3.2	362
25	Atomistic simulations of structures and mechanical properties of polycrystalline diamond: Symmetrical ã€˜001ã€‰ tilt grain boundaries. Physical Review B, 1999, 60, 7043-7052.	3.2	38
26	Molecular Dynamics Simulations of Polymer-Nanotube Composites. Materials Research Society Symposia Proceedings, 1999, 593, 199.	0.1	10
27	Multiscale modeling approach for calculating grain-boundary energies from first principles. Physical Review B, 1998, 57, R3181-R3184.	3.2	46
28	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
29	Atomistic Modeling of Grain Boundary Fracture in Diamond. Materials Research Society Symposia Proceedings, 1998, 539, 319.	0.1	1
30	Detonation of solid O[sub 3]: Effects of void collapse. AIP Conference Proceedings, 1996, , .	0.4	0
31	Ion Beam Damage of Polymer Surfaces: Insights from Molecular-Dynamics Simulation. Materials Research Society Symposia Proceedings, 1996, 438, 491.	0.1	3
32	Coexistence Of Two Carbon Phases At Grain Boundaries In Polycrystalline Diamond. Materials Research Society Symposia Proceedings, 1996, 442, 693.	0.1	4
33	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
34	Molecular Dynamics Simulation of Atomic-Scale Adhesion, Deformation, Friction, and Modification of Diamond Surfaces. , 1995, , 175-181.		0
35	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
36	Chemistry and phase transitions from hypervelocity impacts. International Journal of Quantum Chemistry, 1994, 52, 129-137.	2.0	8

#	Article	IF	Citations
37	Special C44 Isomers. Materials Research Society Symposia Proceedings, 1994, 349, 331.	0.1	1
38	Fullerene/Tubule Based Hollow Carbon Nano-Gears. Materials Research Society Symposia Proceedings, 1994, 349, 283.	0.1	16
39	Molecular Dynamics Simulations of Hypervelocity Buckminsterfullerene Collisions. Materials Research Society Symposia Proceedings, 1994, 359, 199.	0.1	0
40	Molecular dynamics of void collapse mechanisms in shocked media. AIP Conference Proceedings, 1994, , .	0.4	0
41	Detonations at nanometer resolution using molecular dynamics. Physical Review Letters, 1993, 70, 2174-2177.	7.8	137
42	Molecular-dynamics simulations of atomic-scale friction of diamond surfaces. Physical Review B, 1992, 46, 9700-9708.	3.2	250
43	Photoelectron Spectra of C60H36 and C60H60. Materials Research Society Symposia Proceedings, 1992, 247, 351.	0.1	0
44	Dissociative Phase Transitions, Split Shock Waves, Rarefaction Shocks, and Detonations. Materials Research Society Symposia Proceedings, 1992, 296, 123.	0.1	1
45	Molecular Dynamics Simulations of Dimer Opening on a Diamond Â(2x1) Surface. Science, 1992, 255, 835-838.	12.6	201
46	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
47	Energetics of nanoscale graphitic tubules. Physical Review B, 1992, 45, 12592-12595.	3.2	893
48	Relative Energetics of C44 Fullerene Isomers. , 1992, , 1347-1351.		2
49	Split shock waves from molecular dynamics. Physical Review Letters, 1991, 67, 3132-3135.	7.8	57
50	Atomistic Simulation of the Nanoindentation of Diamond and Graphite Surfaces. Materials Research Society Symposia Proceedings, 1991, 239, 573.	0.1	17
51	Local density functional electronic structures of three stable icosahedral fullerenes. The Journal of Physical Chemistry, 1991, 95, 8737-8741.	2.9	92
52	Group-IV covalent clusters:Si45andC44versusSi44andC45. Physical Review B, 1991, 44, 3479-3482.	3.2	26
53	Local-density-functional calculation of photoelectron spectra of fullerenes. Physical Review B, 1991, 43, 14281-14284.	3.2	56
54	Simulations of buckminsterfullerene (C60) collisions with a hydrogen-terminated diamond {111} surface. The Journal of Physical Chemistry, 1991, 95, 7138-7142.	2.9	144

#	Article	IF	Citations
55	Possidle Isomers and Electronic Structure of C60H36. Materials Research Society Symposia Proceedings, 1990, 206, 687.	0.1	3
56	First-Principles Study of Photoexcited Defects in Polysilane Chains. Materials Research Society Symposia Proceedings, 1990, 209, 189.	0.1	0
57	Limits of chemical effects on cold fusion. Journal of Fusion Energy, 1990, 9, 363-366.	1.2	2
58	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
59	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