Arthur F Voter

List of Publications by Year
in descending order

79 papers	8,028 citations	117453 34 h-index	74018 75 g-index
79 all docs	79 docs citations	79 times ranked	4961 citing authors

#	Article	IF	Citations
1	Efficient Annealing of Radiation Damage Near Grain Boundaries via Interstitial Emission. Science, 2010, 327, 1631-1634.	6.0	884
2	Hyperdynamics: Accelerated Molecular Dynamics of Infrequent Events. Physical Review Letters, 1997, 78, 3908-3911.	2.9	873
3	Temperature-accelerated dynamics for simulation of infrequent events. Journal of Chemical Physics, 2000, 112, 9599-9606.	1.2	664
4	Extending the Time Scale in Atomistic Simulation of Materials. Annual Review of Materials Research, 2002, 32, 321-346.	4.3	614
5	A method for accelerating the molecular dynamics simulation of infrequent events. Journal of Chemical Physics, 1997, 106, 4665-4677.	1.2	556
6	Parallel replica method for dynamics of infrequent events. Physical Review B, 1998, 57, R13985-R13988.	1.1	498
7	Classically exact overlayer dynamics: Diffusion of rhodium clusters on Rh(100). Physical Review B, 1986, 34, 6819-6829.	1.1	457
8	Dynamical corrections to transition state theory for multistate systems: Surface selfâ€diffusion in the rareâ€event regime. Journal of Chemical Physics, 1985, 82, 80-92.	1.2	272
9	Synchronization of trajectories in canonical molecular-dynamics simulations: Observation, explanation, and exploitation. Journal of Chemical Physics, 2004, 120, 6363-6374.	1.2	221
10	Highly optimized tight-binding model of silicon. Physical Review B, 1997, 55, 1528-1544.	1.1	212
11	Diffusion mechanisms in Cu grain boundaries. Physical Review B, 2000, 62, 3658-3673.	1.1	197
12	Bad Seeds Sprout Perilous Dynamics: Stochastic Thermostat Induced Trajectory Synchronization in Biomolecules. Journal of Chemical Theory and Computation, 2009, 5, 1624-1631.	2.3	170
13	Highly optimized empirical potential model of silicon. Modelling and Simulation in Materials Science and Engineering, 2000, 8, 825-841.	0.8	151
14	Transition state theory description of surface selfâ€diffusion: Comparison with classical trajectory results. Journal of Chemical Physics, 1984, 80, 5832-5838.	1.2	144
15	Chapter 4 Accelerated Molecular Dynamics Methods: Introduction and Recent Developments. Annual Reports in Computational Chemistry, 2009, , 79-98.	0.9	139
16	Thermostatted molecular dynamics: How to avoid the Toda demon hidden in NosÃ©-Hoover dynamics. Physical Review E, 1995, 52, 2338-2347.	0.8	132
17	Competing Kinetics and He Bubble Morphology in W. Physical Review Letters, 2015, 114, 105502.	2.9	108
18	The generalized resonating valence bond description of cyclobutadiene. Journal of the American Chemical Society, 1986, 108, 2830-2837.	6.6	97

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19	A Monte Carlo method for determining freeâ€energy differences and transition state theory rate constants. Journal of Chemical Physics, 1985, 82, 1890-1899.	1.2	95
20	A method for describing resonance between generalized valence bond wavefunctions. Chemical Physics, 1981, 57, 253-259.	0.9	93
21	Accurate acceleration of kinetic Monte Carlo simulations through the modification of rate constants. Journal of Chemical Physics, 2010, 132, 194101.	1.2	86
22	The parallel replica dynamics method â€“ Coming of age. Computational Materials Science, 2015, 100, 90-103.	1.4	85
23	Molecular-dynamics simulations of two-dimensional materials at high strain rates. Physical Review A, 1992, 45, 8457-8470.	1.0	82
24	Long-Time Dynamics through Parallel Trajectory Splicing. Journal of Chemical Theory and Computation, 2016, 12, 18-28.	2.3	74
25	The generalized resonating valence bond method: Barrier heights in the HF + D and HCl + D exchange reactions. Journal of Chemical Physics, 1981, 75, 3638-3639.	1.2	65
26	Smart Darting Monte Carlo. Journal of Chemical Physics, 2001, 114, 6994-7000.	1.2	60
27	The isotope and temperature dependence of self-diffusion for hydrogen, deuterium, and tritium on Cu(100) in the 100â€“1000 K range. Surface Science, 1985, 155, 687-699.	0.8	55
28	Interatomic Potentials for Atomistic Simulations. MRS Bulletin, 1996, 21, 17-19.	1.7	50
29	The mobility of small vacancy/helium complexes in tungsten and its impact on retention in fusion-relevant conditions. Scientific Reports, 2017, 7, 2522.	1.6	50
30	Molecular dynamics-based ion-surface interaction models for ionized physical vapor deposition feature scale simulations. Applied Physics Letters, 1998, 73, 3860-3862.	1.5	45
31	The Modern Temperature-Accelerated Dynamics Approach. Annual Review of Chemical and Biomolecular Engineering, 2016, 7, 87-110.	3.3	45
32	Reflection and implantation of low energy helium with tungsten surfaces. Journal of Nuclear Materials, 2014, 447, 254-270.	1.3	39
33	Hyper-QC: An accelerated finite-temperature quasicontinuum method using hyperdynamics. Journal of the Mechanics and Physics of Solids, 2014, 63, 94-112.	2.3	38
34	Formation of helium-bubble networks in tungsten. Acta Materialia, 2018, 159, 46-50.	3.8	35
35	Low-Speed Atomistic Simulation of Stickâ€“Slip Friction using Parallel Replica Dynamics. Tribology Letters, 2009, 36, 63-68.	1.2	34
36	Mechanisms and Rates of InterstitialH2Diffusion in CrystallineC60. Physical Review Letters, 2003, 91, 105901.	2.9	32

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37	Local hyperdynamics. Journal of Chemical Physics, 2013, 139, 144110.	1.2	32
38	Surface selfâ€diffusion constants at low temperature: Monte Carlo transition state theory with importance sampling. Journal of Chemical Physics, 1984, 80, 5814-5817.	1.2	28
39	Computing classically exact diffusion constants using short-time trajectories. Physical Review Letters, 1989, 63, 167-170.	2.9	25
40	Low-order moment expansions to tight binding for interatomic potentials: Successes and failures. Physical Review B, 1995, 52, 8766-8775.	1.1	25
41	Parallel replica dynamics with a heterogeneous distribution of barriers: Application ton-hexadecane pyrolysis. Journal of Chemical Physics, 2004, 121, 9808-9819.	1.2	25
42	Thermostating extended Lagrangian Born-Oppenheimer molecular dynamics. Journal of Chemical Physics, 2015, 142, 154120.	1.2	25
43	Compact surface-cluster diffusion by concerted rotation and translation. Physical Review B, 2000, 61, R5125-R5128.	1.1	24
44	Accelerated dynamics simulations of interstitial-cluster growth. Solid State Communications, 2001, 120, 279-282.	0.9	24
45	Atomistic study of the dissolution of small boron interstitial clusters in c-Si. Applied Physics Letters, 2005, 87, 191912.	1.5	24
46	Vacancy Formation and Strain in Low-Temperature<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Cu</mml:mi><mml:mo>/</mml:mo><mml:mi>Cu</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>100</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 367 Td (stretchy="false">)</mml:mo>	2.9	24
47	Understanding the Surface Diffusion Processes during Magnetron Sputter-Deposition of Complex Oxide Mgâ€“Alâ€“O Thin Films. Crystal Growth and Design, 2011, 11, 2553-2558.	1.4	22
48	The Roles of Statics and Dynamics in Determining Transitions Between Atomic Friction Regimes. Tribology Letters, 2011, 42, 99-107.	1.2	22
49	The thermodynamic and kinetic interactions of He interstitial clusters with bubbles in W. Journal of Applied Physics, 2016, 119, .	1.1	21
50	Long-time molecular dynamics simulations on massively parallel platforms: A comparison of parallel replica dynamics and parallel trajectory splicing. Journal of Materials Research, 2018, 33, 813-822.	1.2	21
51	Growth Rate Effects on the Formation of Dislocation Loops Around Deep Helium Bubbles in Tungsten. Fusion Science and Technology, 2017, 71, 1-6.	0.6	20
52	Intraatomic exchange and the violation of Hund's rule in twisted ethylene. Chemical Physics, 1985, 98, 7-14.	0.9	18
53	Hyperdynamics boost factor achievable with an ideal bias potential. Journal of Chemical Physics, 2015, 143, 074113.	1.2	17
54	Convergence of surface diffusion parameters with model crystal size. Surface Science, 1994, 313, 439-447.	0.8	16

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55	Interatomic potential for directional bonding: The rotated-second-moment approximation. Physical Review B, 1991, 43, 12607-12610.	1.1	12
56	TADSim. ACM Transactions on Modeling and Computer Simulation, 2015, 25, 1-26.	0.6	12
57	The effects of cationâ€“anion clustering on defect migration in MgAl₂O₄. Physical Chemistry Chemical Physics, 2016, 18, 19647-19654.	1.3	12
58	Cluster analysis of accelerated molecular dynamics simulations: A case study of the decahedron to icosahedron transition in Pt nanoparticles. Journal of Chemical Physics, 2017, 147, 152717.	1.2	12
59	Discovering mechanisms relevant for radiation damage evolution. Computational Materials Science, 2018, 147, 282-292.	1.4	12
60	Discrete event performance prediction of speculatively parallel temperature-accelerated dynamics. Simulation, 2016, 92, 1065-1086.	1.1	11
61	Reactive Bond-Order Simulations Using Both Spatial and Temporal Approaches to Parallelism. Structural Chemistry, 2004, 15, 479-486.	1.0	10
62	Entropic Stabilization of Nanoscale Voids in Materials under Tension. Physical Review Letters, 2013, 110, 206001.	2.9	10
63	Analysis of Transition State Theory Rates upon Spatial Coarse-Graining. Multiscale Modeling and Simulation, 2015, 13, 890-915.	0.6	9
64	Parallel algorithms for hyperdynamics and local hyperdynamics. Journal of Chemical Physics, 2020, 153, 054116.	1.2	9
65	An Overview of Recent Standard and Accelerated Molecular Dynamics Simulations of Helium Behavior in Tungsten. Materials, 2019, 12, 2500.	1.3	7
66	Structure and mobility of radiation-induced defects in MgO. Journal of Computer-Aided Materials Design, 2007, 14, 183-189.	0.7	6
67	Insights into Microscopic Diffusion Processes at a Solid/Fluid Interface under Supercritical Conditions: A Study of the Aqueous Calcite (101l...4) Surface. Journal of Physical Chemistry C, 2012, 116, 25934-25942.	1.5	6
68	Extending atomistic simulation timescale in solid/liquid systems: Crystal growth from solution by a parallel-replica dynamics and continuum hybrid method. Journal of Chemical Physics, 2014, 140, 044116.	1.2	6
69	Speculation and replication in temperature accelerated dynamics. Journal of Materials Research, 2018, 33, 823-834.	1.2	6
70	Scalable kernel polynomial method for calculating transition rates. Physical Review B, 2013, 87, .	1.1	5
71	Computing long time scale biomolecular dynamics using quasi-stationary distribution kinetic Monte Carlo (QSD-KMC). Journal of Chemical Physics, 2019, 151, 074109.	1.2	4
72	Determining Reaction Mechanisms. , 2005, , 1627-1634.		3

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73	Accelerating ring-polymer molecular dynamics with parallel-replica dynamics. Journal of Chemical Physics, 2016, 144, 244109.	1.2	3
74	Accelerated Molecular Dynamics Methods in a Massively Parallel World. , 2020, , 745-772.		3
75	Failure of 1D Models for Ir Island Diffusion on Ir(111). Physical Review Letters, 2000, 85, 1580-1580.	2.9	2
76	Locally disrupted synchronization in Langevin molecular dynamics. Physical Review E, 2012, 86, 026703.	0.8	2
77	Model description of transition metals using the rotated second moment approximation. Radiation Effects and Defects in Solids, 1994, 129, 45-53.	0.4	1
78	Langevin synchronization in a time-dependent, harmonic basin: An exact solution in 1D. Journal of Chemical Physics, 2018, 148, 084107.	1.2	0
79	Computing Long Time Dynamics using Dynamically Corrected Kinetic Monte Carlo (DC-KMC). Biophysical Journal, 2019, 116, 166a.	0.2	0