

Arthur F Voter

List of Publications by Year in descending order

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79
papers

8,028
citations

117625
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75
g-index

79
all docs

79
docs citations

79
times ranked

4961
citing authors

#	ARTICLE	IF	CITATIONS
1	Parallel algorithms for hyperdynamics and local hyperdynamics. Journal of Chemical Physics, 2020, 153, 054116.	3.0	9
2	Accelerated Molecular Dynamics Methods in a Massively Parallel World. , 2020, , 745-772.		3
3	An Overview of Recent Standard and Accelerated Molecular Dynamics Simulations of Helium Behavior in Tungsten. Materials, 2019, 12, 2500.	2.9	7
4	Computing long time scale biomolecular dynamics using quasi-stationary distribution kinetic Monte Carlo (QSD-KMC). Journal of Chemical Physics, 2019, 151, 074109.	3.0	4
5	Computing Long Time Dynamics using Dynamically Corrected Kinetic Monte Carlo (DC-KMC). Biophysical Journal, 2019, 116, 166a.	0.5	0
6	Speculation and replication in temperature accelerated dynamics. Journal of Materials Research, 2018, 33, 823-834.	2.6	6
7	Discovering mechanisms relevant for radiation damage evolution. Computational Materials Science, 2018, 147, 282-292.	3.0	12
8	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.	2.6	21
9	Langevin synchronization in a time-dependent, harmonic basin: An exact solution in 1D. Journal of Chemical Physics, 2018, 148, 084107.	3.0	0
10	Formation of helium-bubble networks in tungsten. Acta Materialia, 2018, 159, 46-50.	7.9	35
11	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.	3.0	12
12	The mobility of small vacancy/helium complexes in tungsten and its impact on retention in fusion-relevant conditions. Scientific Reports, 2017, 7, 2522.	3.3	50
13	Growth Rate Effects on the Formation of Dislocation Loops Around Deep Helium Bubbles in Tungsten. Fusion Science and Technology, 2017, 71, 1-6.	1.1	20
14	The Modern Temperature-Accelerated Dynamics Approach. Annual Review of Chemical and Biomolecular Engineering, 2016, 7, 87-110.	6.8	45
15	The effects of cation–anion clustering on defect migration in MgAl ₂ O ₄ . Physical Chemistry Chemical Physics, 2016, 18, 19647-19654.	2.8	12
16	The thermodynamic and kinetic interactions of He interstitial clusters with bubbles in W. Journal of Applied Physics, 2016, 119, .	2.5	21
17	Discrete event performance prediction of speculatively parallel temperature-accelerated dynamics. Simulation, 2016, 92, 1065-1086.	1.8	11
18	Accelerating ring-polymer molecular dynamics with parallel-replica dynamics. Journal of Chemical Physics, 2016, 144, 244109.	3.0	3

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19	Long-Time Dynamics through Parallel Trajectory Splicing. Journal of Chemical Theory and Computation, 2016, 12, 18-28.	5.3	74
20	Hyperdynamics boost factor achievable with an ideal bias potential. Journal of Chemical Physics, 2015, 143, 074113.	3.0	17
21	Analysis of Transition State Theory Rates upon Spatial Coarse-Graining. Multiscale Modeling and Simulation, 2015, 13, 890-915.	1.6	9
22	Competing Kinetics and He Bubble Morphology in W. Physical Review Letters, 2015, 114, 105502.	7.8	108
23	TADSim. ACM Transactions on Modeling and Computer Simulation, 2015, 25, 1-26.	0.8	12
24	The parallel replica dynamics method “Coming of age. Computational Materials Science, 2015, 100, 90-103.	3.0	85
25	Thermostating extended Lagrangian Born-Oppenheimer molecular dynamics. Journal of Chemical Physics, 2015, 142, 154120.	3.0	25
26	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.	3.0	6
27	Hyper-QC: An accelerated finite-temperature quasicontinuum method using hyperdynamics. Journal of the Mechanics and Physics of Solids, 2014, 63, 94-112.	4.8	38
28	Reflection and implantation of low energy helium with tungsten surfaces. Journal of Nuclear Materials, 2014, 447, 254-270.	2.7	39
29	Scalable kernel polynomial method for calculating transition rates. Physical Review B, 2013, 87, .	3.2	5
30	Entropic Stabilization of Nanoscale Voids in Materials under Tension. Physical Review Letters, 2013, 110, 206001.	7.8	10
31	Local hyperdynamics. Journal of Chemical Physics, 2013, 139, 144110.	3.0	32
32	Locally disrupted synchronization in Langevin molecular dynamics. Physical Review E, 2012, 86, 026703.	2.1	2
33	Insights into Microscopic Diffusion Processes at a Solid/Fluid Interface under Supercritical Conditions: A Study of the Aqueous Calcite (101...4) Surface. Journal of Physical Chemistry C, 2012, 116, 25934-25942.	3.1	6
34	Understanding the Surface Diffusion Processes during Magnetron Sputter-Deposition of Complex Oxide MgO Thin Films. Crystal Growth and Design, 2011, 11, 2553-2558.	3.0	22
35	The Roles of Statics and Dynamics in Determining Transitions Between Atomic Friction Regimes. Tribology Letters, 2011, 42, 99-107.	2.6	22
36	Efficient Annealing of Radiation Damage Near Grain Boundaries via Interstitial Emission. Science, 2010, 327, 1631-1634.	12.6	884

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37	Accurate acceleration of kinetic Monte Carlo simulations through the modification of rate constants. Journal of Chemical Physics, 2010, 132, 194101.	3.0	86
38	Low-Speed Atomistic Simulation of Stickâ€“Slip Friction using Parallel Replica Dynamics. Tribology Letters, 2009, 36, 63-68.	2.6	34
39	Bad Seeds Sprout Perilous Dynamics: Stochastic Thermostat Induced Trajectory Synchronization in Biomolecules. Journal of Chemical Theory and Computation, 2009, 5, 1624-1631.	5.3	170
40	Chapter 4 Accelerated Molecular Dynamics Methods: Introduction and Recent Developments. Annual Reports in Computational Chemistry, 2009, , 79-98.	1.7	139
41	Vacancy Formation and Strain in Low-Temperature<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></mml:mo><mml:mn>100</mml:mn><mml:mo>T_j</mml:mo>ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 567 Td (stretchy="false">	7.8	24
42	Structure and mobility of radiation-induced defects in MgO. Journal of Computer-Aided Materials Design, 2007, 14, 183-189.	0.7	6
43	Atomistic study of the dissolution of small boron interstitial clusters in c-Si. Applied Physics Letters, 2005, 87, 191912.	3.3	24
44	Determining Reaction Mechanisms. , 2005, , 1627-1634.		3
45	Parallel replica dynamics with a heterogeneous distribution of barriers: Application ton-hexadecane pyrolysis. Journal of Chemical Physics, 2004, 121, 9808-9819.	3.0	25
46	Reactive Bond-Order Simulations Using Both Spatial and Temporal Approaches to Parallelism. Structural Chemistry, 2004, 15, 479-486.	2.0	10
47	Synchronization of trajectories in canonical molecular-dynamics simulations: Observation, explanation, and exploitation. Journal of Chemical Physics, 2004, 120, 6363-6374.	3.0	221
48	Mechanisms and Rates of InterstitialH2Diffusion in CrystallineC60. Physical Review Letters, 2003, 91, 105901.	7.8	32
49	Extending the Time Scale in Atomistic Simulation of Materials. Annual Review of Materials Research, 2002, 32, 321-346.	9.3	614
50	Smart Darting Monte Carlo. Journal of Chemical Physics, 2001, 114, 6994-7000.	3.0	60
51	Accelerated dynamics simulations of interstitial-cluster growth. Solid State Communications, 2001, 120, 279-282.	1.9	24
52	Temperature-accelerated dynamics for simulation of infrequent events. Journal of Chemical Physics, 2000, 112, 9599-9606.	3.0	664
53	Failure of 1D Models for Ir Island Diffusion on Ir(111). Physical Review Letters, 2000, 85, 1580-1580.	7.8	2
54	Highly optimized empirical potential model of silicon. Modelling and Simulation in Materials Science and Engineering, 2000, 8, 825-841.	2.0	151

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55	Compact surface-cluster diffusion by concerted rotation and translation. Physical Review B, 2000, 61, R5125-R5128.	3.2	24
56	Diffusion mechanisms in Cu grain boundaries. Physical Review B, 2000, 62, 3658-3673.	3.2	197
57	Parallel replica method for dynamics of infrequent events. Physical Review B, 1998, 57, R13985-R13988.	3.2	498
58	Molecular dynamics-based ion-surface interaction models for ionized physical vapor deposition feature scale simulations. Applied Physics Letters, 1998, 73, 3860-3862.	3.3	45
59	Hyperdynamics: Accelerated Molecular Dynamics of Infrequent Events. Physical Review Letters, 1997, 78, 3908-3911.	7.8	873
60	Highly optimized tight-binding model of silicon. Physical Review B, 1997, 55, 1528-1544.	3.2	212
61	A method for accelerating the molecular dynamics simulation of infrequent events. Journal of Chemical Physics, 1997, 106, 4665-4677.	3.0	556
62	Interatomic Potentials for Atomistic Simulations. MRS Bulletin, 1996, 21, 17-19.	3.5	50
63	Thermostatted molecular dynamics: How to avoid the Toda demon hidden in Nosé-Hoover dynamics. Physical Review E, 1995, 52, 2338-2347.	2.1	132
64	Low-order moment expansions to tight binding for interatomic potentials: Successes and failures. Physical Review B, 1995, 52, 8766-8775.	3.2	25
65	Model description of transition metals using the rotated second moment approximation. Radiation Effects and Defects in Solids, 1994, 129, 45-53.	1.2	1
66	Convergence of surface diffusion parameters with model crystal size. Surface Science, 1994, 313, 439-447.	1.9	16
67	Molecular-dynamics simulations of two-dimensional materials at high strain rates. Physical Review A, 1992, 45, 8457-8470.	2.5	82
68	Interatomic potential for directional bonding: The rotated-second-moment approximation. Physical Review B, 1991, 43, 12607-12610.	3.2	12
69	Computing classically exact diffusion constants using short-time trajectories. Physical Review Letters, 1989, 63, 167-170.	7.8	25
70	Classically exact overlayer dynamics: Diffusion of rhodium clusters on Rh(100). Physical Review B, 1986, 34, 6819-6829.	3.2	457
71	The generalized resonating valence bond description of cyclobutadiene. Journal of the American Chemical Society, 1986, 108, 2830-2837.	13.7	97
72	Intraatomic exchange and the violation of Hund's rule in twisted ethylene. Chemical Physics, 1985, 98, 7-14.	1.9	18

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73	A Monte Carlo method for determining free-energy differences and transition state theory rate constants. Journal of Chemical Physics, 1985, 82, 1890-1899.	3.0	95
74	The isotope and temperature dependence of self-diffusion for hydrogen, deuterium, and tritium on Cu(100) in the 100–1000 K range. Surface Science, 1985, 155, 687-699.	1.9	55
75	Dynamical corrections to transition state theory for multistate systems: Surface self-diffusion in the rare-event regime. Journal of Chemical Physics, 1985, 82, 80-92.	3.0	272
76	Surface self-diffusion constants at low temperature: Monte Carlo transition state theory with importance sampling. Journal of Chemical Physics, 1984, 80, 5814-5817.	3.0	28
77	Transition state theory description of surface self-diffusion: Comparison with classical trajectory results. Journal of Chemical Physics, 1984, 80, 5832-5838.	3.0	144
78	A method for describing resonance between generalized valence bond wavefunctions. Chemical Physics, 1981, 57, 253-259.	1.9	93
79	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.	3.0	65