

Normand Mousseau

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

189
papers

6,109
citations

44
h-index

72
g-index

209
ext. papers

6,591
ext. citations

4.3
avg, IF

5.92
L-index

#	Paper	IF	Citations
189	Activation/Relaxation Technique: An efficient way to find minima and saddle points of potential energy surfaces. <i>Computational Materials Science</i> , 2022 , 209, 111363	3.2	0
188	Polyphenol-Peptide Interactions in Mitigation of Alzheimer's Disease: Role of Biosurface-Induced Aggregation. <i>Journal of Alzheimer's Disease</i> , 2021 , 81, 33-55	4.3	0
187	Corilagin and 1,3,6-Tri-galloyl-D-glucose: potential inhibitors of SARS-CoV-2 variants. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 14873-14888	3.6	3
186	The energy landscape governs ductility in disordered materials. <i>Materials Horizons</i> , 2021 , 8, 1242-1252	14.4	7
185	Capturing the Iron Carburization Mechanisms from the Surface to Bulk. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 28569-28579	3.8	6
184	Identifying flow defects in amorphous alloys using machine learning outlier detection methods. <i>Scripta Materialia</i> , 2020 , 186, 185-189	5.6	17
183	Order and disorder at the C-face of SiC: A hybrid surface reconstruction. <i>Applied Physics Letters</i> , 2020 , 116, 141605	3.4	1
182	Simulation of Single Particle Displacement Damage in Si ₃ N ₄ Alloys Interaction of Primary Particles With the Material and Generation of the Damage Structure. <i>IEEE Transactions on Nuclear Science</i> , 2020 , 67, 1273-1283	1.7	3
181	Off-Lattice Kinetic Monte Carlo Methods 2020 , 715-743		2
180	Atomistic Kinetic Monte Carlo and Solute Effects 2020 , 2437-2456		
179	Kinetic Monte Carlo Simulations of Irradiation Effects 2020 , 754-778		4
178	Finding Reaction Pathways and Transition States: r-ARTn and d-ARTn as an Efficient and Versatile Alternative to String Approaches. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 6726-6734	6.4	9
177	Enthalpy-entropy compensation of atomic diffusion originates from softening of low frequency phonons. <i>Nature Communications</i> , 2020 , 11, 3977	17.4	7
176	Elucidating the role of extended surface defects at Fe surfaces on CO adsorption and dissociation. <i>Applied Surface Science</i> , 2019 , 491, 792-798	6.7	7
175	Is Hydrogen Diffusion along Grain Boundaries Fast or Slow? Atomistic Origin and Mechanistic Modeling. <i>Physical Review Letters</i> , 2019 , 122, 215501	7.4	16
174	Off-Lattice Kinetic Monte Carlo Methods 2019 , 1-29		2
173	ART_data_analyzer: Automating parallelized computations to study the evolution of materials. <i>SoftwareX</i> , 2019 , 9, 238-243	2.7	5

172	Mitigating Alzheimer's Disease with Natural Polyphenols: A Review. <i>Current Alzheimer Research</i> , 2019 , 16, 529-543	3	27
171	. <i>IEEE Transactions on Nuclear Science</i> , 2018 , 65, 724-731	1.7	8
170	Carbon diffusion paths and segregation at high-angle tilt grain boundaries in α -Fe studied by using a kinetic activation-relation technique. <i>Physical Review B</i> , 2018 , 97,	3.3	11
169	Interaction between interstitial carbon atoms and a $\langle 111 \rangle$ self-interstitial atoms loop in an iron matrix: a combined DFT, off lattice KMC and MD study. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 335901	1.8	1
168	Study of point defects diffusion in nickel using kinetic activation-relaxation technique. <i>Acta Materialia</i> , 2018 , 144, 679-690	8.4	16
167	Atomistic Kinetic Monte Carlo and Solute Effects 2018 , 1-20		1
166	Long-time point defect diffusion in ordered nickel-based binary alloys: How small kinetic differences can lead to completely long-time structural evolution. <i>Materialia</i> , 2018 , 4, 575-584	3.2	6
165	Off-Lattice Kinetic Monte Carlo Methods 2018 , 1-29		
164	Benchmarking the performance of plane-wave vs. localized orbital basis set methods in DFT modeling of metal surface: a case study for Fe-(110). <i>Journal of Computational Science</i> , 2018 , 29, 163-167	2.4	4
163	Carbon adsorption on and diffusion through the Fe(110) surface and in bulk: Developing a new strategy for the use of empirical potentials in complex material set-ups. <i>Physica Status Solidi (B): Basic Research</i> , 2017 , 254, 1600408	1.3	13
162	Algorithmic developments of the kinetic activation-relaxation technique: Accessing long-time kinetics of larger and more complex systems. <i>Journal of Chemical Physics</i> , 2017 , 147, 152712	3.9	10
161	Strain-driven diffusion process during silicon oxidation investigated by coupling density functional theory and activation relaxation technique. <i>Journal of Chemical Physics</i> , 2017 , 147, 054701	3.9	3
160	Structural and thermodynamical properties of early human amylin oligomers using replica exchange molecular dynamics: mutation effect of three key residues F15, H18 and F23. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 31290-31299	3.6	8
159	Energy landscape and diffusion kinetics of lithiated silicon: A kinetic activation-relaxation technique study. <i>Physical Review B</i> , 2017 , 96,	3.3	9
158	The role of emerging grain boundary at iron surface, temperature and hydrogen on metal dusting initiation. <i>Acta Materialia</i> , 2017 , 135, 340-347	8.4	8
157	Diffusion mechanisms of C in 100, 110 and 111 Fe surfaces studied using kinetic activation-relaxation technique. <i>Acta Materialia</i> , 2017 , 136, 303-314	8.4	11
156	Simulation of Single Particle Displacement Damage in Silicon Part II: Generation and Long-Time Relaxation of Damage Structure. <i>IEEE Transactions on Nuclear Science</i> , 2017 , 64, 141-148	1.7	39
155	Stimulating a Canadian narrative for climate. <i>Facets</i> , 2017 , 2, 131-149	2.3	3

154	Na ₃ Fe ₂ (SO ₄) ₂ (SO ₃ N) as a potential high capacity cathode material. <i>Materials Science and Engineering B: Solid-State Materials for Advanced Technology</i> , 2016 , 211, 185-190	3.1	1
153	Free-Energy Landscape of the Amino-Terminal Fragment of Huntingtin in Aqueous Solution. <i>Biophysical Journal</i> , 2016 , 110, 1075-88	2.9	11
152	Diffusion properties of Fe ²⁺ systems studied by using kinetic activation-relaxation technique. <i>Computational Materials Science</i> , 2016 , 112, 96-106	3.2	17
151	Insights on finite size effects in ab initio study of CO adsorption and dissociation on Fe 110 surface. <i>Journal of Applied Physics</i> , 2016 , 120, 055301	2.5	14
150	Influence of surface vacancy defects on the carburisation of Fe 110 surface by carbon monoxide. <i>Journal of Chemical Physics</i> , 2016 , 145, 044710	3.9	10
149	Diffusion of point defects in crystalline silicon using the kinetic activation-relaxation technique method. <i>Physical Review B</i> , 2015 , 91,	3.3	25
148	Following atomistic kinetics on experimental timescales with the kinetic Activation-Relaxation Technique. <i>Computational Materials Science</i> , 2015 , 100, 111-123	3.2	21
147	Strong Long-Range Relaxations of Structural Defects in Graphene Simulated Using a New Semiempirical Potential. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 9646-9655	3.8	18
146	Probing the Huntingtin 1-17 membrane anchor on a phospholipid bilayer by using all-atom simulations. <i>Biophysical Journal</i> , 2015 , 108, 1187-98	2.9	16
145	Probing Potential Energy Surface Exploration Strategies for Complex Systems. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 1970-7	6.4	1
144	Amyloid β Protein and Alzheimer's Disease: When Computer Simulations Complement Experimental Studies. <i>Chemical Reviews</i> , 2015 , 115, 3518-63	68.1	426
143	Aggregation process of A β -40 with non-A β amyloid component of β -synuclein. <i>Journal of Physics: Conference Series</i> , 2015 , 640, 012008	0.3	
142	A novel intercalation cathode material for sodium-based batteries. <i>Electrochemistry Communications</i> , 2015 , 52, 9-12	5.1	1
141	Distinct helix propensities and membrane interactions of human and rat IAPP(1-19) monomers in anionic lipid bilayers. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 3366-76	3.4	25
140	The OPEP protein model: from single molecules, amyloid formation, crowding and hydrodynamics to DNA/RNA systems. <i>Chemical Society Reviews</i> , 2014 , 43, 4871-93	58.5	118
139	Atomistic mechanisms of huntingtin N-terminal fragment insertion on a phospholipid bilayer revealed by molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 1409-27	4.2	10
138	Strain effects and intermixing at the Si surface: Importance of long-range elastic corrections in first-principles calculations. <i>Physical Review B</i> , 2014 , 90,	3.3	8
137	Understanding long-time vacancy aggregation in iron: A kinetic activation-relaxation technique study. <i>Physical Review B</i> , 2014 , 90,	3.3	33

136	Early oligomerization stages for the non-amyloid component of β -synuclein amyloid. <i>Journal of Chemical Physics</i> , 2014 , 141, 135103	3.9	11
135	Oligomerization of Huntingtin N-Terminal Fragment on a Phospholipid Bilayer Revealed by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2014 , 106, 99a-100a	2.9	1
134	Kinetics of Amyloid Growth. <i>Molecular Medicine and Molecular Biology</i> , 2013 , 209-237		1
133	Contribution of vacancies to relaxation in amorphous materials: A kinetic activation-relaxation technique study. <i>Physical Review B</i> , 2013 , 87,	3.3	30
132	Replenish and relax: explaining logarithmic annealing in ion-implanted c-Si. <i>Physical Review Letters</i> , 2013 , 111, 105502	7.4	29
131	Long-time relaxation of ion-bombarded silicon studied with the kinetic activation-relaxation technique: Microscopic description of slow aging in a disordered system. <i>Physical Review B</i> , 2013 , 88,	3.3	24
130	Tunable magnetic states in hexagonal boron nitride sheets. <i>Applied Physics Letters</i> , 2012 , 101, 132405	3.4	25
129	Molecular dynamics simulations of the bacterial ABC transporter SAV1866 in the closed form. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 2934-42	3.4	34
128	Structures of A β 17-42 trimers in isolation and with five small-molecule drugs using a hierarchical computational procedure. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 8412-22	3.4	92
127	All-atom stability and oligomerization simulations of polyglutamine nanotubes with and without the 17-amino-acid N-terminal fragment of the Huntingtin protein. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 12168-79	3.4	11
126	Large loop conformation sampling using the activation relaxation technique, ART-nouveau method. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012 , 80, 1883-94	4.2	4
125	Distinct dimerization for various alloforms of the amyloid-beta protein: A β (1-40), A β (1-42), and A β (1-40)(D23N). <i>Journal of Physical Chemistry B</i> , 2012 , 116, 4043-55	3.4	90
124	Kinetics of amyloid aggregation: a study of the GNNQQNY prion sequence. <i>PLoS Computational Biology</i> , 2012 , 8, e1002782	5	35
123	Comment on "Mechanism of void nucleation and growth in bcc Fe: atomistic simulations at experimental time scales". <i>Physical Review Letters</i> , 2012 , 108, 219601; author reply 219602	7.4	17
122	Understanding the EF-hand closing pathway using non-biased interatomic potentials. <i>Journal of Chemical Physics</i> , 2012 , 136, 035101	3.9	14
121	First stages of silicon oxidation with the activation relaxation technique. <i>Physical Review B</i> , 2012 , 86,	3.3	6
120	Optimization of the Kinetic Activation-Relaxation Technique, an off-lattice and self-learning kinetic Monte-Carlo method. <i>Journal of Physics: Conference Series</i> , 2012 , 341, 012007	0.3	14
119	The Activation-Relaxation Technique: ART Nouveau and Kinetic ART. <i>Journal of Atomic, Molecular, and Optical Physics</i> , 2012 , 2012, 1-14		41

118	Holographic multiscale method used with non-biased atomistic forcefields for simulation of large transformations in protein. <i>Journal of Physics: Conference Series</i> , 2012 , 341, 012015	0.3	1
117	Energy landscape of small clusters of self-interstitial dumbbells in iron. <i>Physical Review B</i> , 2011 , 83,	3.3	69
116	Kinetic activation-relaxation technique. <i>Physical Review E</i> , 2011 , 84, 046704	2.4	108
115	Use of Umbrella Sampling to Calculate the Entrance/Exit Pathway for Z-Pro-Prolinal Inhibitor in Prolyl Oligopeptidase. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 1583-94	6.4	27
114	Distinct Morphologies for Amyloid Beta Protein Monomer: A β -40, A β -42, and A β -40(D23N). <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2584-92	6.4	71
113	Structure and thermodynamics of amylin dimer studied by Hamiltonian-temperature replica exchange molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 3146-54	3.4	61
112	Amorphous silicon under mechanical shear deformations: Shear velocity and temperature effects. <i>Physical Review B</i> , 2011 , 83,	3.3	7
111	Crystallization of amorphous silicon induced by mechanical shear deformations. <i>Physical Review B</i> , 2011 , 84,	3.3	15
110	A multiscale approach to characterize the early aggregation steps of the amyloid-forming peptide GNNQQNY from the yeast prion sup-35. <i>PLoS Computational Biology</i> , 2011 , 7, e1002051	5	68
109	Optimized energy landscape exploration using the ab initio based activation-relaxation technique. <i>Journal of Chemical Physics</i> , 2011 , 135, 034102	3.9	72
108	Spontaneous formation of polyglutamine nanotubes with molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2010 , 132, 165102	3.9	22
107	Evolution of the potential-energy surface of amorphous silicon. <i>Physical Review Letters</i> , 2010 , 105, 045503	3.4	46
106	Effect of the disulfide bond on the monomeric structure of human amylin studied by combined Hamiltonian and temperature replica exchange molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 7071-7	3.4	60
105	Thermodynamics and dynamics of amyloid peptide oligomerization are sequence dependent. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 75, 954-63	4.2	102
104	Structures and thermodynamics of Alzheimer's amyloid-beta A β (16-35) monomer and dimer by replica exchange molecular dynamics simulations: implication for full-length A β fibrillation. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 7668-75	3.4	92
103	Replica exchange molecular dynamics simulations of coarse-grained proteins in implicit solvent. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 267-74	3.4	67
102	The beta-strand-loop-beta-strand conformation is marginally populated in beta2-microglobulin (20-41) peptide in solution as revealed by replica exchange molecular dynamics simulations. <i>Biophysical Journal</i> , 2008 , 95, 510-7	2.9	11
101	Self-assembly of the beta2-microglobulin NHVTL SQ peptide using a coarse-grained protein model reveals a beta-barrel species. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 4410-8	3.4	71

100	The complex folding pathways of protein A suggest a multiple-funnelled energy landscape. <i>Journal of Chemical Physics</i> , 2008 , 128, 045101	3.9	16
99	Energy landscapes of the monomer and dimer of the Alzheimer's peptide Abeta(1-28). <i>Journal of Chemical Physics</i> , 2008 , 128, 125108	3.9	24
98	Role of the region 23-28 in Abeta fibril formation: insights from simulations of the monomers and dimers of Alzheimer's peptides Abeta40 and Abeta42. <i>Current Alzheimer Research</i> , 2008 , 5, 244-50	3	91
97	Numerical characterization of the Ga interstitial self-diffusion mechanisms in GaAs. <i>Journal of Applied Physics</i> , 2008 , 103, 113502	2.5	9
96	Kinetic activation-relaxation technique: An off-lattice self-learning kinetic Monte Carlo algorithm. <i>Physical Review B</i> , 2008 , 78,	3.3	114
95	Self-assembly of amyloid-forming peptides by molecular dynamics simulations. <i>Frontiers in Bioscience - Landmark</i> , 2008 , 13, 5681-92	2.8	37
94	Exploring energy landscapes of protein folding and aggregation. <i>Frontiers in Bioscience - Landmark</i> , 2008 , 13, 4495-516	2.8	12
93	Ab initio study of the diffusion mechanisms of gallium in a silicon matrix. <i>European Physical Journal B</i> , 2008 , 64, 165-172	1.2	11
92	Ab-initio simulations of self-diffusion mechanisms in semiconductors. <i>Physica B: Condensed Matter</i> , 2007 , 401-402, 658-661	2.8	4
91	Ab initio characterization of arsenic vacancy diffusion pathways in GaAs with SIEST-A-RT. <i>Applied Physics A: Materials Science and Processing</i> , 2007 , 86, 309-312	2.6	7
90	Probing amyloid fibril formation of the NFGAIL peptide by computer simulations. <i>Journal of Chemical Physics</i> , 2007 , 126, 065101	3.9	29
89	Sampling small-scale and large-scale conformational changes in proteins and molecular complexes. <i>Journal of Chemical Physics</i> , 2007 , 126, 105101	3.9	7
88	Gallium self-interstitial relaxation in GaAs: An ab initio characterization. <i>Physical Review B</i> , 2007 , 76,	3.3	19
87	Self-organized criticality in the intermediate phase of rigidity percolation. <i>Physical Review E</i> , 2007 , 75, 056108	2.4	26
86	Computational simulations of the early steps of protein aggregation. <i>Prion</i> , 2007 , 1, 3-8	2.3	59
85	Coarse-grained protein molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2007 , 126, 025101	3.9	84
84	The conformations of the amyloid-beta (21-30) fragment can be described by three families in solution. <i>Journal of Chemical Physics</i> , 2006 , 125, 084911	3.9	60
83	Self-organization with equilibration: a model for the intermediate phase in rigidity percolation. <i>Physical Review E</i> , 2006 , 74, 016116	2.4	54

82	Thermally activated charge reversibility of gallium vacancies in GaAs. <i>Journal of Applied Physics</i> , 2006 , 100, 083521	2.5	11
81	Charge-dependent migration pathways for the Ga vacancy in GaAs. <i>Physical Review B</i> , 2006 , 74,	3.3	8
80	Exploiting memory in event-based simulations. <i>Journal of Non-Crystalline Solids</i> , 2006 , 352, 4424-4429	3.9	3
79	ARTIST: an activated method in internal coordinate space for sampling protein energy landscapes. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006 , 63, 967-75	4.2	13
78	Structures of soluble amyloid oligomers from computer simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006 , 65, 180-91	4.2	52
77	Aggregating the amyloid Abeta(11-25) peptide into a four-stranded beta-sheet structure. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006 , 65, 877-88	4.2	21
76	Following the aggregation of amyloid-forming peptides by computer simulations. <i>Journal of Chemical Physics</i> , 2005 , 122, 174904	3.9	57
75	Exploring the early steps of amyloid peptide aggregation by computers. <i>Accounts of Chemical Research</i> , 2005 , 38, 885-91	24.3	81
74	Self-vacancies in gallium arsenide: An ab initio calculation. <i>Physical Review B</i> , 2005 , 71,	3.3	51
73	Liquid-liquid phase transition in Stillinger-Weber silicon. <i>Journal of Physics Condensed Matter</i> , 2005 , 17, 2269-2279	1.8	35
72	Activated sampling in complex materials at finite temperature: the properly obeying probability activation-relaxation technique. <i>Journal of Chemical Physics</i> , 2005 , 123, 244707	3.9	4
71	Nucleation and crystallization process of silicon using the Stillinger-Weber potential. <i>Physical Review B</i> , 2005 , 71,	3.3	34
70	Navigation and analysis of the energy landscape of small proteins using the activation-relaxation technique. <i>Physical Biology</i> , 2005 , 2, S101-7	3	6
69	Exploring the early steps of aggregation of amyloid-forming peptide KFFE. <i>Journal of Physics Condensed Matter</i> , 2004 , 16, S5047-S5054	1.8	10
68	Binary continuous random networks. <i>Journal of Physics Condensed Matter</i> , 2004 , 16, S5183-S5190	1.8	8
67	Pathway complexity of Alzheimer's beta-amyloid Abeta16-22 peptide assembly. <i>Structure</i> , 2004 , 12, 1245-55	12.1	
66	Complex folding pathways in a simple beta-hairpin. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 56, 464-74	4.2	76
65	In silico assembly of Alzheimer's Abeta16-22 peptide into beta-sheets. <i>Journal of the American Chemical Society</i> , 2004 , 126, 11509-16	16.4	125

64	Sampling the self-assembly pathways of KFFE hexamers. <i>Biophysical Journal</i> , 2004 , 87, 3648-56	2.9	69
63	Sampling the diffusion paths of a neutral vacancy in silicon with quantum mechanical calculations. <i>Physical Review B</i> , 2004 , 70,	3.3	70
62	Exploring the Folding and Aggregation Mechanisms of Amyloid-Forming Peptides by Computer Simulations 2004 , 379-381		
61	Numerical Studies Of The Dynamics Of Silicon: Relaxation, Nucleation And Energy Landscape. <i>Materials Research Society Symposia Proceedings</i> , 2003 , 762, 1111		
60	Relationship between dynamical heterogeneities and stretched exponential relaxation. <i>Physical Review E</i> , 2003 , 68, 041110	2.4	14
59	Sampling the complex energy landscape of a simple hairpin. <i>Journal of Chemical Physics</i> , 2003 , 119, 6403-6406	3.9	54
58	Energy landscape of relaxed amorphous silicon. <i>Physical Review B</i> , 2003 , 68,	3.3	35
57	Characterization of the stretched-exponential trap-time distributions in one-dimensional coupled map lattices. <i>Physical Review E</i> , 2002 , 66, 066205	2.4	8
56	Exploring the energy landscape of proteins: A characterization of the activation-relaxation technique. <i>Journal of Chemical Physics</i> , 2002 , 117, 11379-11387	3.9	46
55	Comment on Boson peak in amorphous silicon: A numerical study <i>Physical Review B</i> , 2002 , 66,	3.3	5
54	Stretched-exponential dynamics in a chain of coupled chaotic oscillators. <i>Europhysics Letters</i> , 2002 , 60, 827-833	1.6	8
53	Recent developments in the study of continuous random networks. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , 2002 , 82, 171-183		7
52	Crystallization study of model tetrahedral semiconductors. <i>Journal of Physics Condensed Matter</i> , 2002 , 14, 6627-6638	1.8	15
51	Sampling activated mechanisms in proteins with the activation-relaxation technique. <i>Journal of Molecular Graphics and Modelling</i> , 2001 , 19, 78-86	2.8	25
50	MODELS OF PARACRYSTALLINE SILICON WITH A DEFECT-FREE BANDGAP. <i>International Journal of Modern Physics B</i> , 2001 , 15, 3253-3257	1.1	7
49	Diffusion in Lennard-Jones Glasses: Simulation Studies of the Activation Parameters for Collective Mechanisms. <i>Defect and Diffusion Forum</i> , 2001 , 194-199, 855-860	0.7	1
48	Simulating Diffusion at Low Temperatures in Binary Lennard-Jones Glasses: The Activation-Relaxation Technique. <i>Defect and Diffusion Forum</i> , 2001 , 194-199, 775-788	0.7	1
47	Efficient tight-binding Monte Carlo structural sampling of complex materials. <i>Europhysics Letters</i> , 2001 , 56, 427-433	1.6	6

46	Realistic models of paracrystalline silicon. <i>Physical Review B</i> , 2001 , 63,	3.3	48
45	Fast bond-transposition algorithms for generating covalent amorphous structures. <i>Current Opinion in Solid State and Materials Science</i> , 2001 , 5, 497-502	12	9
44	The activation-relaxation technique: an efficient algorithm for sampling energy landscapes. <i>Computational Materials Science</i> , 2001 , 20, 285-292	3.2	33
43	Fitting the Stillinger-Weber potential to amorphous silicon. <i>Journal of Non-Crystalline Solids</i> , 2001 , 282, 248-255	3.9	136
42	Basic mechanisms of structural relaxation and diffusion in amorphous silicon. <i>Materials Research Society Symposia Proceedings</i> , 2001 , 664, 2811		1
41	Characterization of the Activation-Relaxation Technique: Recent Results on Models of Amorphous Silicon. <i>Materials Research Society Symposia Proceedings</i> , 2001 , 677, 841		1
40	Numerical studies of the vibrational isocoordinate rule in chalcogenide glasses. <i>European Physical Journal B</i> , 2000 , 17, 667-671	1.2	5
39	High-quality continuous random networks. <i>Physical Review B</i> , 2000 , 62, 4985-4990	3.3	206
38	Approximate ab initio calculations of electronic structure of amorphous silicon. <i>Physical Review B</i> , 2000 , 62, 15307-15310	3.3	26
37	Elementary mechanisms governing the dynamics of silica. <i>Journal of Chemical Physics</i> , 2000 , 112, 960-964	3.9	24
36	Optimal activation and diffusion paths of perfect events in amorphous silicon. <i>Physical Review B</i> , 2000 , 62, 15680-15685	3.3	16
35	Activated mechanisms in amorphous silicon: An activation-relaxation-technique study. <i>Physical Review B</i> , 2000 , 61, 1898-1906	3.3	68
34	Dynamics of lennard-jones clusters: A characterization of the activation-relaxation technique. <i>Physical Review E</i> , 2000 , 62, 7723-8	2.4	199
33	Dependence of the vibrational spectra of amorphous silicon on the defect concentration and ring distribution. <i>Journal of Physics Condensed Matter</i> , 1999 , 11, 9647-9658	1.8	30
32	Exploring structural mechanisms in disordered materials using the activation-relaxation technique. <i>Computer Physics Communications</i> , 1999 , 121-122, 206-209	4.2	4
31	Exploring high-dimensional energy landscapes. <i>Computing in Science and Engineering</i> , 1999 , 1, 74-80, 82	1.5	14
30	Tight-binding molecular-dynamics studies of defects and disorder in covalently bonded materials. <i>Computational Materials Science</i> , 1998 , 12, 210-241	3.2	23
29	Surface diffusion coefficients by thermodynamic integration: Cu on Cu(100). <i>Physical Review B</i> , 1998 , 58, 12667-12670	3.3	40

28	Traveling through potential energy landscapes of disordered materials: The activation-relaxation technique. <i>Physical Review E</i> , 1998 , 57, 2419-2424	2.4	182
27	Identification of Relaxation and Diffusion Mechanisms in Amorphous Silicon. <i>Physical Review Letters</i> , 1998 , 81, 1865-1868	7.4	55
26	Comment on Role of Lattice Vibrations in Adatom Diffusion <i>Physical Review Letters</i> , 1998 , 80, 203-203	7.4	14
25	Multiple phase changes induced by frustration in randomly connected cellular automata. <i>Journal of Physics A</i> , 1997 , 30, 2995-3002		
24	Comment on Systematic approach to generate near-perfect periodic continuous random network models: Application to amorphous Si ₃ N ₄ <i>Physical Review B</i> , 1997 , 56, 14190-14191	3.3	1
23	Structural, electronic, and dynamical properties of amorphous gallium arsenide: A comparison between two topological models. <i>Physical Review B</i> , 1997 , 56, 9461-9468	3.3	22
22	sAvalanche distribution in the Feder and Feder model: Effects of quenched disorder. <i>Physical Review E</i> , 1997 , 55, 3682-3685	2.4	
21	Topology of Amorphous Tetrahedral Semiconductors on Intermediate Length Scales. <i>Physical Review Letters</i> , 1997 , 78, 1484-1487	7.4	57
20	Strain broadening of the magnetization steps in diluted magnetic semiconductors. <i>Physical Review B</i> , 1997 , 56, 13094-13102	3.3	6
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