

Normand Mousseau

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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	Amyloid β Protein and Alzheimer's Disease: When Computer Simulations Complement Experimental Studies. <i>Chemical Reviews</i> , 2015 , 115, 3518-63	68.1	426
188	Event-Based Relaxation of Continuous Disordered Systems. <i>Physical Review Letters</i> , 1996 , 77, 4358-4361	7.4	354
187	High-quality continuous random networks. <i>Physical Review B</i> , 2000 , 62, 4985-4990	3.3	206
186	Dynamics of lennard-jones clusters: A characterization of the activation-relaxation technique. <i>Physical Review E</i> , 2000 , 62, 7723-8	2.4	199
185	Traveling through potential energy landscapes of disordered materials: The activation-relaxation technique. <i>Physical Review E</i> , 1998 , 57, 2419-2424	2.4	182
184	Fitting the Stillinger-Weber potential to amorphous silicon. <i>Journal of Non-Crystalline Solids</i> , 2001 , 282, 248-255	3.9	136
183	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
182	Pathway complexity of Alzheimer's beta-amyloid Abeta16-22 peptide assembly. <i>Structure</i> , 2004 , 12, 1245-55	5.5	121
181	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
180	Kinetic activation-relaxation technique: An off-lattice self-learning kinetic Monte Carlo algorithm. <i>Physical Review B</i> , 2008 , 78,	3.3	114
179	Kinetic activation-relaxation technique. <i>Physical Review E</i> , 2011 , 84, 046704	2.4	108
178	Thermodynamics and dynamics of amyloid peptide oligomerization are sequence dependent. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 75, 954-63	4.2	102
177	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
176	Structures and thermodynamics of Alzheimer's amyloid-beta Abeta(16-35) monomer and dimer by replica exchange molecular dynamics simulations: implication for full-length Abeta fibrillation. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 7668-75	3.4	92
175	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
174	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
173	Coarse-grained protein molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2007 , 126, 025101	3.9	84

172	Exploring the early steps of amyloid peptide aggregation by computers. <i>Accounts of Chemical Research</i> , 2005 , 38, 885-91	24.3	81
171	Complex folding pathways in a simple beta-hairpin. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004 , 56, 464-74	4.2	76
170	Optimized energy landscape exploration using the ab initio based activation-relaxation technique. <i>Journal of Chemical Physics</i> , 2011 , 135, 034102	3.9	72
169	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
168	Self-assembly of the beta2-microglobulin NHVTLsq 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
167	Sampling the diffusion paths of a neutral vacancy in silicon with quantum mechanical calculations. <i>Physical Review B</i> , 2004 , 70,	3.3	70
166	Energy landscape of small clusters of self-interstitial dumbbells in iron. <i>Physical Review B</i> , 2011 , 83,	3.3	69
165	Sampling the self-assembly pathways of KFFE hexamers. <i>Biophysical Journal</i> , 2004 , 87, 3648-56	2.9	69
164	A multiscale approach to characterize the early aggregation steps of the amyloid-forming peptide GNNQNY from the yeast prion sup-35. <i>PLoS Computational Biology</i> , 2011 , 7, e1002051	5	68
163	Activated mechanisms in amorphous silicon: An activation-relaxation-technique study. <i>Physical Review B</i> , 2000 , 61, 1898-1906	3.3	68
162	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
161	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
160	Length mismatch in random semiconductor alloys. III. Crystalline and amorphous SiGe. <i>Physical Review B</i> , 1992 , 46, 15887-15893	3.3	61
159	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
158	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
157	Computational simulations of the early steps of protein aggregation. <i>Prion</i> , 2007 , 1, 3-8	2.3	59
156	Topology of Amorphous Tetrahedral Semiconductors on Intermediate Length Scales. <i>Physical Review Letters</i> , 1997 , 78, 1484-1487	7.4	57
155	Following the aggregation of amyloid-forming peptides by computer simulations. <i>Journal of Chemical Physics</i> , 2005 , 122, 174904	3.9	57

154	Identification of Relaxation and Diffusion Mechanisms in Amorphous Silicon. <i>Physical Review Letters</i> , 1998 , 81, 1865-1868	7.4	55
153	Self-organization with equilibration: a model for the intermediate phase in rigidity percolation. <i>Physical Review E</i> , 2006 , 74, 016116	2.4	54
152	Sampling the complex energy landscape of a simple hairpin. <i>Journal of Chemical Physics</i> , 2003 , 119, 6403-6406	3.9	54
151	Structures of soluble amyloid oligomers from computer simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006 , 65, 180-91	4.2	52
150	Self-vacancies in gallium arsenide: An ab initio calculation. <i>Physical Review B</i> , 2005 , 71,	3.3	51
149	Synchronization by Disorder in Coupled Systems. <i>Physical Review Letters</i> , 1996 , 77, 968-971	7.4	49
148	Realistic models of paracrystalline silicon. <i>Physical Review B</i> , 2001 , 63,	3.3	48
147	Evolution of the potential-energy surface of amorphous silicon. <i>Physical Review Letters</i> , 2010 , 105, 045503	3.4	46
146	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
145	The Activation-Relaxation Technique: ART Nouveau and Kinetic ART. <i>Journal of Atomic, Molecular, and Optical Physics</i> , 2012 , 2012, 1-14		41
144	Length distributions in metallic alloys. <i>Physical Review B</i> , 1992 , 45, 2015-2022	3.3	41
143	Surface diffusion coefficients by thermodynamic integration: Cu on Cu(100). <i>Physical Review B</i> , 1998 , 58, 12667-12670	3.3	40
142	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
141	Self-assembly of amyloid-forming peptides by molecular dynamics simulations. <i>Frontiers in Bioscience - Landmark</i> , 2008 , 13, 5681-92	2.8	37
140	Structural model for crystalline and amorphous Si-Ge alloys. <i>Physical Review B</i> , 1993 , 48, 5172-5178	3.3	37
139	Dynamical models of hydrogenated amorphous silicon. <i>Physical Review B</i> , 1991 , 43, 9810-9817	3.3	36
138	Kinetics of amyloid aggregation: a study of the GNNQQNY prion sequence. <i>PLoS Computational Biology</i> , 2012 , 8, e1002782	5	35
137	Energy landscape of relaxed amorphous silicon. <i>Physical Review B</i> , 2003 , 68,	3.3	35

136	Liquid-liquid phase transition in Stillinger-Weber silicon. <i>Journal of Physics Condensed Matter</i> , 2005 , 17, 2269-2279	1.8	35
135	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
134	Nucleation and crystallization process of silicon using the Stillinger-Weber potential. <i>Physical Review B</i> , 2005 , 71,	3.3	34
133	Understanding long-time vacancy aggregation in iron: A kinetic activation-relaxation technique study. <i>Physical Review B</i> , 2014 , 90,	3.3	33
132	The activation-relaxation technique: an efficient algorithm for sampling energy landscapes. <i>Computational Materials Science</i> , 2001 , 20, 285-292	3.2	33
131	Contribution of vacancies to relaxation in amorphous materials: A kinetic activation-relaxation technique study. <i>Physical Review B</i> , 2013 , 87,	3.3	30
130	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
129	Replenish and relax: explaining logarithmic annealing in ion-implanted c-Si. <i>Physical Review Letters</i> , 2013 , 111, 105502	7.4	29
128	Probing amyloid fibril formation of the NFGAIL peptide by computer simulations. <i>Journal of Chemical Physics</i> , 2007 , 126, 065101	3.9	29
127	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
126	Mitigating Alzheimer's Disease with Natural Polyphenols: A Review. <i>Current Alzheimer Research</i> , 2019 , 16, 529-543	3	27
125	Self-organized criticality in the intermediate phase of rigidity percolation. <i>Physical Review E</i> , 2007 , 75, 056108	2.4	26
124	Approximate ab initio calculations of electronic structure of amorphous silicon. <i>Physical Review B</i> , 2000 , 62, 15307-15310	3.3	26
123	Diffusion of point defects in crystalline silicon using the kinetic activation-relaxation technique method. <i>Physical Review B</i> , 2015 , 91,	3.3	25
122	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
121	Tunable magnetic states in hexagonal boron nitride sheets. <i>Applied Physics Letters</i> , 2012 , 101, 132405	3.4	25
120	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
119	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

118	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
117	Elementary mechanisms governing the dynamics of silica. <i>Journal of Chemical Physics</i> , 2000 , 112, 960-964	3.9	24
116	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
115	Spontaneous formation of polyglutamine nanotubes with molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2010 , 132, 165102	3.9	22
114	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
113	Following atomistic kinetics on experimental timescales with the kinetic ActivationRelaxation Technique. <i>Computational Materials Science</i> , 2015 , 100, 111-123	3.2	21
112	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
111	Computer models for amorphous silicon hydrides. <i>Physical Review B</i> , 1990 , 41, 3702-3707	3.3	21
110	Photometric and polarimetric variability and mass-loss rate of the massive binary Wolf-Rayet star HDE 311884 (WN6 + O5: V). <i>Astrophysical Journal</i> , 1990 , 350, 767	4.7	20
109	Gallium self-interstitial relaxation in GaAs: An ab initio characterization. <i>Physical Review B</i> , 2007 , 76,	3.3	19
108	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
107	Identifying flow defects in amorphous alloys using machine learning outlier detection methods. <i>Scripta Materialia</i> , 2020 , 186, 185-189	5.6	17
106	Diffusion properties of Fe α systems studied by using kinetic activationRelaxation technique. <i>Computational Materials Science</i> , 2016 , 112, 96-106	3.2	17
105	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
104	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
103	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
102	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
101	Optimal activation and diffusion paths of perfect events in amorphous silicon. <i>Physical Review B</i> , 2000 , 62, 15680-15685	3.3	16

100	Study of point defects diffusion in nickel using kinetic activation-relaxation technique. <i>Acta Materialia</i> , 2018 , 144, 679-690	8.4	16
99	Crystallization of amorphous silicon induced by mechanical shear deformations. <i>Physical Review B</i> , 2011 , 84,	3.3	15
98	Crystallization study of model tetrahedral semiconductors. <i>Journal of Physics Condensed Matter</i> , 2002 , 14, 6627-6638	1.8	15
97	Understanding the EF-hand closing pathway using non-biased interatomic potentials. <i>Journal of Chemical Physics</i> , 2012 , 136, 035101	3.9	14
96	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
95	Relationship between dynamical heterogeneities and stretched exponential relaxation. <i>Physical Review E</i> , 2003 , 68, 041110	2.4	14
94	Comment on Role of Lattice Vibrations in Adatom Diffusion \square <i>Physical Review Letters</i> , 1998 , 80, 203-203	7.4	14
93	Exploring high-dimensional energy landscapes. <i>Computing in Science and Engineering</i> , 1999 , 1, 74-80, 82	1.5	14
92	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
91	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
90	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
89	Exploring energy landscapes of protein folding and aggregation. <i>Frontiers in Bioscience - Landmark</i> , 2008 , 13, 4495-516	2.8	12
88	Carbon diffusion paths and segregation at high-angle tilt grain boundaries in δ Fe studied by using a kinetic activation-relation technique. <i>Physical Review B</i> , 2018 , 97,	3.3	11
87	Free-Energy Landscape of the Amino-Terminal Fragment of Huntingtin in Aqueous Solution. <i>Biophysical Journal</i> , 2016 , 110, 1075-88	2.9	11
86	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
85	Early oligomerization stages for the non-amyloid component of β synuclein amyloid. <i>Journal of Chemical Physics</i> , 2014 , 141, 135103	3.9	11
84	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
83	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

82	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
81	Thermally activated charge reversibility of gallium vacancies in GaAs. <i>Journal of Applied Physics</i> , 2006 , 100, 083521	2.5	11
80	Onset of avalanches in granular media. <i>Physical Review E</i> , 1994 , 49, 4712-4715	2.4	11
79	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
78	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
77	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
76	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
75	Energy landscape and diffusion kinetics of lithiated silicon: A kinetic activation-relaxation technique study. <i>Physical Review B</i> , 2017 , 96,	3.3	9
74	Numerical characterization of the Ga interstitial self-diffusion mechanisms in GaAs. <i>Journal of Applied Physics</i> , 2008 , 103, 113502	2.5	9
73	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
72	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
71	. <i>IEEE Transactions on Nuclear Science</i> , 2018 , 65, 724-731	1.7	8
70	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
69	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
68	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
67	Charge-dependent migration pathways for the Ga vacancy in GaAs. <i>Physical Review B</i> , 2006 , 74,	3.3	8
66	Binary continuous random networks. <i>Journal of Physics Condensed Matter</i> , 2004 , 16, S5183-S5190	1.8	8
65	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

64	Stretched-exponential dynamics in a chain of coupled chaotic oscillators. <i>Europhysics Letters</i> , 2002 , 60, 827-833	1.6	8
63	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
62	Amorphous silicon under mechanical shear deformations: Shear velocity and temperature effects. <i>Physical Review B</i> , 2011 , 83,	3.3	7
61	Randomly connected cellular automata: a search for critical connectivities. <i>Europhysics Letters</i> , 1996 , 33, 509-514	1.6	7
60	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
59	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
58	MODELS OF PARACRYSTALLINE SILICON WITH A DEFECT-FREE BANDGAP. <i>International Journal of Modern Physics B</i> , 2001 , 15, 3253-3257	1.1	7
57	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
56	Recent developments in the study of continuous random networks		7
55	Enthalpy-entropy compensation of atomic diffusion originates from softening of low frequency phonons. <i>Nature Communications</i> , 2020 , 11, 3977	17.4	7
54	The energy landscape governs ductility in disordered materials. <i>Materials Horizons</i> , 2021 , 8, 1242-1252	14.4	7
53	Capturing the Iron Carburization Mechanisms from the Surface to Bulk. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 28569-28579	3.8	6
52	First stages of silicon oxidation with the activation relaxation technique. <i>Physical Review B</i> , 2012 , 86,	3.3	6
51	Strain broadening of the magnetization steps in diluted magnetic semiconductors. <i>Physical Review B</i> , 1997 , 56, 13094-13102	3.3	6
50	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
49	Efficient tight-binding Monte Carlo structural sampling of complex materials. <i>Europhysics Letters</i> , 2001 , 56, 427-433	1.6	6
48	Size-mismatch disorder at the surface of semiconductors. <i>Physical Review B</i> , 1995 , 52, 2660-2667	3.3	6
47	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

46	ART_data_analyzer: Automating parallelized computations to study the evolution of materials. <i>SoftwareX</i> , 2019 , 9, 238-243	2.7	5
45	Comment on Boson peak in amorphous silicon: A numerical study <i>Physical Review B</i> , 2002 , 66,	3.3	5
44	Numerical studies of the vibrational isocoordinate rule in chalcogenide glasses. <i>European Physical Journal B</i> , 2000 , 17, 667-671	1.2	5
43	Frustration-Induced Phase Transition in High-Dimensional Deterministic Cellular Automata. <i>Europhysics Letters</i> , 1994 , 28, 551-556	1.6	5
42	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
41	Ab-initio simulations of self-diffusion mechanisms in semiconductors. <i>Physica B: Condensed Matter</i> , 2007 , 401-402, 658-661	2.8	4
40	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
39	Exploring structural mechanisms in disordered materials using the activation-relaxation technique. <i>Computer Physics Communications</i> , 1999 , 121-122, 206-209	4.2	4
38	Kinetic Monte Carlo Simulations of Irradiation Effects 2020 , 754-778		4
37	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 ^{3,4}		4
36	Simulation of Single Particle Displacement Damage in Si ₂ Ge _x 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
35	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
34	On the phase diagram of frustrated (quasi-)periodic cellular automata. <i>Journal of Physics A</i> , 1996 , 29, 3021-3036		3
33	Exploiting memory in event-based simulations. <i>Journal of Non-Crystalline Solids</i> , 2006 , 352, 4424-4429	3.9	3
32	Length mismatch in random semiconductor alloys. IV. General multinary compounds. <i>Physical Review B</i> , 1995 , 52, 17191-17198	3.3	3
31	Stimulating a Canadian narrative for climate. <i>Facets</i> , 2017 , 2, 131-149	2.3	3
30	Corilagin and 1,3,6-Tri-galloy- β -D-glucose: potential inhibitors of SARS-CoV-2 variants. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 14873-14888	3.6	3
29	Off-Lattice Kinetic Monte Carlo Methods 2019 , 1-29		2

28	Off-Lattice Kinetic Monte Carlo Methods 2020 , 715-743		2
27	Probing Potential Energy Surface Exploration Strategies for Complex Systems. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 1970-7	6.4	1
26	Order and disorder at the C-face of SiC: A hybrid surface reconstruction. <i>Applied Physics Letters</i> , 2020 , 116, 141605	3.4	1
25	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
24	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
23	A novel intercalation cathode material for sodium-based batteries. <i>Electrochemistry Communications</i> , 2015 , 52, 9-12	5.1	1
22	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
21	Kinetics of Amyloid Growth. <i>Molecular Medicine and Medicinal</i> , 2013 , 209-237		1
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