

Simulations on the Thermal Decomposition of a Poly(di ReaxFF Reactive Force Field

Journal of the American Chemical Society

127, 7192-7202

DOI: 10.1021/ja050980t

Citation Report

#	ARTICLE	IF	CITATIONS
2	Formation of water at a Pt(111) surface: A study using the reactive force field (ReaxFF). Materials Research Society Symposia Proceedings, 2005, 900, 1.	0.1	4
3	Atomistic-Scale Simulations of the Initial Chemical Events in the Thermal Initiation of Triacetoneperoxide. Journal of the American Chemical Society, 2005, 127, 11053-11062.	13.7	147
4	Multi-paradigm multi-scale simulations for fuel cell catalysts and membranes. Molecular Simulation, 2006, 32, 251-268.	2.0	117
5	Dynamics of the Dissociation of Hydrogen on Stepped Platinum Surfaces Using the ReaxFF Reactive Force Field. Journal of Physical Chemistry B, 2006, 110, 4274-4282.	2.6	116
6	Atomistic and continuum modeling of mechanical properties of collagen: Elasticity, fracture, and self-assembly. Journal of Materials Research, 2006, 21, 1947-1961.	2.6	256
7	Multiparadigm Modeling of Dynamical Crack Propagation in Silicon Using a Reactive Force Field. Physical Review Letters, 2006, 96, 095505.	7.8	214
8	Selective attachment of multi-walled carbon nanotubes on poly(dimethyl siloxane)substrates. Macromolecular Research, 2006, 14, 579-583.	2.4	4
9	Split charge equilibration method with correct dissociation limits. Journal of Chemical Physics, 2007, 127, 224103.	3.0	44
10	Hierarchical chemo-nanomechanics of proteins: entropic elasticity, protein unfolding and molecular fracture. Journal of Mechanics of Materials and Structures, 2007, 2, 1019-1057.	0.6	28
11	Silicones. , 2007, , 651-697.		16
12	Some Simulations and Theoretical Studies on Poly(dimethylsiloxane). Polymer Reviews, 2007, 47, 463-485.	10.9	24
13	Computational Parameters. , 2007, , 59-65.		3
14	Two theoretical simulations of hydrocarbons thermal cracking: Reactive force field and density functional calculations. Computational and Theoretical Chemistry, 2008, 852, 62-70.	1.5	16
15	Synthesis and specific features of the structure of the mixed anionic six-coordinate silicon complexes with the (O,O)-dianionic and (C,O)-monoanionic chelate ligands. Russian Chemical Bulletin, 2008, 57, 2093-2100.	1.5	8
16	Theoretical and computational hierarchical nanomechanics of protein materials: Deformation and fracture. Progress in Materials Science, 2008, 53, 1101-1241.	32.8	168
17	Complexation of tris(pentafluorophenyl)silanes with neutral Lewis bases. Journal of Organometallic Chemistry, 2008, 693, 1005-1019.	1.8	19
18	A scalable parallel algorithm for large-scale reactive force-field molecular dynamics simulations. Computer Physics Communications, 2008, 178, 73-87.	7.5	75
19	Fragment distribution of thermal decomposition for PS and PET with QMD calculations by considering the excited and charged model molecules. Applied Surface Science, 2008, 255, 856-859.	6.1	7

#	ARTICLE	IF	CITATIONS
20	Equilibrium Molecular Dynamics Simulations. , 2009, , 255-290.		9
21	Collagen. , 2008, , .		394
22	ReaxFF Reactive Force Field for Solid Oxide Fuel Cell Systems with Application to Oxygen Ion Transport in Yttria-Stabilized Zirconia. Journal of Physical Chemistry A, 2008, 112, 3133-3140.	2.5	88
23	ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation. Journal of Physical Chemistry A, 2008, 112, 1040-1053.	2.5	1,892
24	Molecular Modeling of Complex Chemical Systems. Journal of the American Chemical Society, 2008, 130, 16824-16827.	13.7	58
25	Development of a Q2MM Force Field for the Asymmetric Rhodium Catalyzed Hydrogenation of Enamides. Journal of Chemical Theory and Computation, 2008, 4, 1313-1323.	5.3	63
26	Development and Application of a ReaxFF Reactive Force Field for Oxidative Dehydrogenation on Vanadium Oxide Catalysts. Journal of Physical Chemistry C, 2008, 112, 14645-14654.	3.1	138
27	ReaxFF Reactive Force Field for the Y-Doped BaZrO ₃ Proton Conductor with Applications to Diffusion Rates for Multigranular Systems. Journal of Physical Chemistry A, 2008, 112, 11414-11422.	2.5	95
28	Effect of ion species on apatite-forming ability of silicone elastomer substrates irradiated by cluster ion beams. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2009, 161, 155-159.	3.5	0
29	Induction of bioactivity on silicone elastomer by simultaneous irradiation of oxygen cluster and monomer ion beams. Acta Biomaterialia, 2009, 5, 621-627.	8.3	3
30	Nonisothermal Degradation of Zetaplus Impression Material: Kinetic Aspects. Industrial & Engineering Chemistry Research, 2009, 48, 7044-7053.	3.7	6
31	Molecular Dynamics Simulation of the Low-Temperature Partial Oxidation of CH ₄ . Journal of Physical Chemistry A, 2009, 113, 1539-1547.	2.5	43
32	Simulating the Initial Stage of Phenolic Resin Carbonization via the ReaxFF Reactive Force Field. Journal of Physical Chemistry A, 2009, 113, 6891-6894.	2.5	107
33	Thermal decomposition process in algaenan of Botryococcus braunii race L. Part 2: Molecular dynamics simulations using the ReaxFF reactive force field. Organic Geochemistry, 2009, 40, 416-427.	1.8	100
34	Early maturation processes in coal. Part 2: Reactive dynamics simulations using the ReaxFF reactive force field on Morwell Brown coal structures. Organic Geochemistry, 2009, 40, 1195-1209.	1.8	183
35	Initiation Mechanisms and Kinetics of Pyrolysis and Combustion of JP-10 Hydrocarbon Jet Fuel. Journal of Physical Chemistry A, 2009, 113, 1740-1746.	2.5	213
36	General formulation of pressure and stress tensor for arbitrary many-body interaction potentials under periodic boundary conditions. Journal of Chemical Physics, 2009, 131, 154107.	3.0	707
37	Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2009, 113, 10619-10640.	2.5	257

#	ARTICLE	IF	CITATIONS
39	Development and Validation of a ReaxFF Reactive Force Field for Cu Cation/Water Interactions and Copper Metal/Metal Oxide/Metal Hydroxide Condensed Phases. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9507-9514.	2.5	156
40	Structural and morphological modification of PDMS thick film surfaces by ion implantation with the formation of strain-induced buckling domains. <i>Acta Materialia</i> , 2010, 58, 1861-1867.	7.9	11
41	Structural evolution during the reduction of chemically derived graphene oxide. <i>Nature Chemistry</i> , 2010, 2, 581-587.	13.6	1,573
42	Stability and Formation Mechanisms of Carbonyl- and Hydroxyl-Decorated Holes in Graphene Oxide. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12053-12061.	3.1	129
43	Molecular dynamics simulations of stability of metal-organic frameworks against H ₂ O using the ReaxFF reactive force field. <i>Chemical Communications</i> , 2010, 46, 5713.	4.1	121
44	Development of a ReaxFF Reactive Force Field for Aqueous Chloride and Copper Chloride. <i>Journal of Physical Chemistry A</i> , 2010, 114, 3556-3568.	2.5	55
45	Microfabricated Gas Chromatography Columns With Monolayer-Protected Gold Stationary Phases. <i>Journal of Microelectromechanical Systems</i> , 2010, 19, 294-304.	2.5	36
46	Development of a Reactive Force Field for Iron-Oxyhydroxide Systems. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6298-6307.	2.5	199
47	Reactive Molecular Dynamics Studies of DMMP Adsorption and Reactivity on Amorphous Silica Surfaces. <i>Journal of Physical Chemistry C</i> , 2010, 114, 18894-18902.	3.1	61
49	Atomistic Modeling of the Decomposition of Charring Ablators. , 2010, , .		2
50	Thermally Stable Transparent Sol-Gel Based Siloxane Hybrid Material with High Refractive Index for Light Emitting Diode (LED) Encapsulation. <i>Chemistry of Materials</i> , 2010, 22, 3549-3555.	6.7	175
51	ReaxFF Reactive Force Field Development and Applications for Molecular Dynamics Simulations of Ammonia Borane Dehydrogenation and Combustion. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5485-5492.	2.5	172
52	Development and Validation of ReaxFF Reactive Force Field for Hydrocarbon Chemistry Catalyzed by Nickel. <i>Journal of Physical Chemistry C</i> , 2010, 114, 4939-4949.	3.1	288
53	<i>Colloquium</i> : Failure of molecules, bones, and the Earth itself. <i>Reviews of Modern Physics</i> , 2010, 82, 1459-1487.	45.6	42
54	Mechanism and Kinetics for the Initial Steps of Pyrolysis and Combustion of 1,6-Dicyclopropane-2,4-hexyne from ReaxFF Reactive Dynamics. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4941-4950.	2.5	103
55	Using a Reactive Force Field To Correlate Mobilities Obtained from Solid-State ¹³ C NMR on Mesoporous Silica Nanoparticle Systems. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16333-16339.	3.1	19
56	First-Principles-Based Multiscale, Multiparadigm Molecular Mechanics and Dynamics Methods for Describing Complex Chemical Processes. <i>Topics in Current Chemistry</i> , 2011, 307, 1-42.	4.0	9
57	Maskless direct micro-structuring of PDMS by femtosecond laser localized rapid curing. <i>Journal of Micromechanics and Microengineering</i> , 2011, 21, 075018.	2.6	19

#	ARTICLE	IF	CITATIONS
58	Development and Application of a ReaxFF Reactive Force Field for Hydrogen Combustion. Journal of Physical Chemistry A, 2011, 115, 960-972.	2.5	100
59	ReaxFF- <i>lj</i> : Correction of the ReaxFF Reactive Force Field for London Dispersion, with Applications to the Equations of State for Energetic Materials. Journal of Physical Chemistry A, 2011, 115, 11016-11022.	2.5	401
60	Dynamic bond-order force field. Journal of Computational Electronics, 2011, 10, 2-20.	2.5	7
61	Strategies for modeling diverse chemical reactions in molecular dynamics simulations of cluster bombardment. Surface and Interface Analysis, 2011, 43, 126-128.	1.8	1
62	Reactive molecular dynamics simulation and chemical kinetic modeling of pyrolysis and combustion of n-dodecane. Combustion and Flame, 2011, 158, 217-226.	5.2	196
63	Multi-scale simulations of in-depth pyrolysis of charring ablative thermal protection material. Computers and Fluids, 2011, 45, 191-196.	2.5	14
64	Modeling initial stage of phenolic pyrolysis: Graphitic precursor formation and interfacial effects. Polymer, 2011, 52, 577-585.	3.8	71
65	Assessing the effect of molecular weight on the kinetics of backbone scission reactions in polyethylene using Reactive Molecular Dynamics. Polymer, 2011, 52, 3104-3111.	3.8	24
66	Thermal decomposition of a honeycomb-network sheet: A molecular dynamics simulation study. Journal of Chemical Physics, 2012, 137, 054901.	3.0	2
67	Force-induced breakdown of flexible polymerized membrane. Physical Review E, 2012, 85, 021805.	2.1	4
68	Multiscale, Multiparadigm Modeling for Nanosystems Characterization and Design. The Electrical Engineering Handbook, 2012, , 935-982.	0.2	0
69	Molecular Dynamics Simulations in Polymer Science. , 2012, , 417-460.		12
70	Ab initio quantum chemical and ReaxFF-based study of the intramolecular iminium \rightleftharpoons enamine conversion in a proline-catalyzed reaction. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9
71	Development of a ReaxFF Reactive Force Field for Ettringite and Study of its Mechanical Failure Modes from Reactive Dynamics Simulations. Journal of Physical Chemistry A, 2012, 116, 3918-3925.	2.5	79
72	Oxidation of Silicon Carbide by O ₂ and H ₂ O: A ReaxFF Reactive Molecular Dynamics Study, Part I. Journal of Physical Chemistry C, 2012, 116, 16111-16121.	3.1	177
73	Chemomechanics control of tearing paths in graphene. Physical Review B, 2012, 85, .	3.2	33
74	Classical Reactive Molecular Dynamics Implementations: State of the Art. ChemPhysChem, 2012, 13, 1127-1151.	2.1	73
75	Parallel reactive molecular dynamics: Numerical methods and algorithmic techniques. Parallel Computing, 2012, 38, 245-259.	2.1	716

#	ARTICLE	IF	CITATIONS
76	Parameterization of a reactive force field using a Monte Carlo algorithm. <i>Journal of Computational Chemistry</i> , 2013, 34, 1143-1154.	3.3	74
77	Particle adsorption at polydimethylsiloxane (PDMS)/water interfaces in the presence of a cross-linking reaction. <i>Journal of Colloid and Interface Science</i> , 2013, 400, 70-77.	9.4	5
78	Vibrational spectroscopic study of poly(dimethylsiloxane)-ZnO nanocomposites. <i>Vibrational Spectroscopy</i> , 2013, 68, 1-10.	2.2	20
79	Rupture Dynamics of Macromolecules. <i>Lecture Notes in Applied and Computational Mechanics</i> , 2013, , 1-42.	2.2	0
80	Algorithms of GPU-enabled reactive force field (ReaxFF) molecular dynamics. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 41, 1-11.	2.4	79
81	Theoretical Simulations of Structure and X-ray Photoelectron Spectra of Glycine and Diglycine Adsorbed on Cu(110). <i>Langmuir</i> , 2013, 29, 10194-10204.	3.5	11
82	A polarizable reactive force field for water to enable molecular dynamics simulations of proton transport. <i>Journal of Chemical Physics</i> , 2013, 138, 174502.	3.0	8
83	Exploring the conformational and reactive dynamics of biomolecules in solution using an extended version of the glycine reactive force field. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15062.	2.8	111
84	Self-weakening in lithiated graphene electrodes. <i>Chemical Physics Letters</i> , 2013, 563, 58-62.	2.6	33
85	Development of the ReaxFF reactive force field for aluminum-molybdenum alloy. <i>Journal of Materials Research</i> , 2013, 28, 1155-1164.	2.6	10
86	Oxygen Interactions with Silica Surfaces: Coupled Cluster and Density Functional Investigation and the Development of a New ReaxFF Potential. <i>Journal of Physical Chemistry C</i> , 2013, 117, 258-269.	3.1	74
87	Development of TiO ₂ and TiO ₂ /Fe-based polymeric nanocomposites by single-step laser pyrolysis. <i>Applied Surface Science</i> , 2013, 278, 305-312.	6.1	6
88	Nanoscale heat transfer from computation to experiment. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3389.	2.8	218
89	Fracture Mechanisms in Organic-Rich Shales: Role of Kerogen. , 2013, , .		27
90	Reactive Potentials for Advanced Atomistic Simulations. <i>Annual Review of Materials Research</i> , 2013, 43, 109-129.	9.3	184
91	Toward a Process-Based Molecular Model of SiC Membranes. 1. Development of a Reactive Force Field. <i>Journal of Physical Chemistry C</i> , 2013, 117, 3308-3319.	3.1	39
92	Tribochemistry of Phosphoric Acid Sheared between Quartz Surfaces: A Reactive Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 25604-25614.	3.1	55
93	A Reactive Molecular Dynamics Study of <i>n</i> -Heptane Pyrolysis at High Temperature. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3266-3278.	2.5	105

#	ARTICLE	IF	CITATIONS
94	High-Temperature Oxidation of SiC-Based Composite: Rate Constant Calculation from ReaxFF MD Simulations, Part II. Journal of Physical Chemistry C, 2013, 117, 5014-5027.	3.1	26
95	Reactive Molecular Dynamics Simulation on Thermal Decomposition of n-Heptane. Chinese Journal of Chemical Physics, 2013, 26, 211-219.	1.3	5
96	Computational chemistry studies of phenolic resin. , 2013, , .		1
97	Detailed Temperature-dependent Study of n-Heptane Pyrolysis at High Temperature. Chinese Journal of Chemical Physics, 2013, 26, 329-336.	1.3	11
98	Neutral-cluster implantation in polymers by computer experiments. Journal of Applied Physics, 2013, 113, .	2.5	13
99	Study of the Thermal Decomposition of PFPEs Lubricants on a Thin DLC Film Using Finitely Extensible Nonlinear Elastic Potential Based Molecular Dynamics Simulation. Journal of Nanotechnology, 2014, 2014, 1-15.	3.4	6
100	IR and Py-GC/MS spectral simulation of polymer film by quantum chemical and quantum molecular dynamics calculations using the polymer models. Russian Journal of Physical Chemistry A, 2014, 88, 2370-2379.	0.6	2
101	Design and synthesis of non-crystallizable, low-T _g polysiloxane elastomers with functional epoxy groups through anionic copolymerization and subsequent epoxidation. RSC Advances, 2014, 4, 31249-31260.	3.6	29
102	Theoretical Chemistry in Belgium. Highlights in Theoretical Chemistry, 2014, , .	0.0	1
103	Predicting Thermo-Mechanical Response of Crosslinked Epoxy using ReaxFF. , 2014, , .		0
104	Reactive force field for electrophilic substitution at an aromatic system in twin polymerization. Chemical Physics, 2014, 440, 119-126.	1.9	14
105	PuReMD-GPU: A reactive molecular dynamics simulation package for GPUs. Journal of Computational Physics, 2014, 272, 343-359.	3.8	47
106	Phenomenological and chemomechanical modeling of the thermomechanical stability of liquid silicone rubbers. Polymer Degradation and Stability, 2014, 99, 290-297.	5.8	16
107	Predicting mechanical response of crosslinked epoxy using ReaxFF. Chemical Physics Letters, 2014, 591, 175-178.	2.6	133
108	Surface Chemistry and Atomic-Scale Reconstruction of Kerogen-Silica Composites. Journal of Physical Chemistry C, 2014, 118, 2429-2438.	3.1	29
109	Characterization of silicon species issued from PDMS degradation under thermal cracking of hydrocarbons: Part 2 - Liquid samples analysis by a multi-technical approach based on gas chromatography and mass spectrometry. Fuel, 2014, 116, 478-489.	6.4	16
110	A molecular based kinetic study on the thermal decomposition of poly-1-methyl styrene. Polymer Degradation and Stability, 2014, 110, 415-421.	5.8	8
111	A coarse-grained molecular dynamics reactive Monte Carlo approach to simulate hyperbranched polycondensation. RSC Advances, 2014, 4, 56625-56636.	3.6	11

#	ARTICLE	IF	CITATIONS
112	Stability of CH ₃ molecules trapped on hydrogenated sites of graphene. <i>Physica B: Condensed Matter</i> , 2014, 455, 60-65.	2.7	7
113	Coarse-Grained Modeling of Peptidic/PDMS Triblock Morphology. <i>Journal of Physical Chemistry B</i> , 2014, 118, 13718-13728.	2.6	11
114	Influence of vacancy defects on the thermal stability of silicene: a reactive molecular dynamics study. <i>RSC Advances</i> , 2014, 4, 1133-1137.	3.6	66
115	Reaction analysis and visualization of ReaxFF molecular dynamics simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 53, 13-22.	2.4	79
116	Parallel Optimization of a Reactive Force Field for Polycondensation of Alkoxysilanes. <i>Journal of Physical Chemistry B</i> , 2014, 118, 10966-10978.	2.6	37
117	Shock initiated thermal and chemical responses of HMX crystal from ReaxFF molecular dynamics simulation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 13914.	2.8	44
118	Large-Scale Reactive Molecular Dynamics Simulation and Kinetic Modeling of High-Temperature Pyrolysis of the <i>Gloeocapsomorpha prisca</i> Microfossils. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6302-6315.	2.6	22
119	Laser-Induced Sub-millisecond Heating Reveals Distinct Tertiary Ester Cleavage Reaction Pathways in a Photolithographic Resist Polymer. <i>ACS Nano</i> , 2014, 8, 5746-5756.	14.6	23
120	The Mitigation Effect of Synthetic Polymers on Initiation Reactivity of CL-20: Physical Models and Chemical Pathways of Thermolysis. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22881-22895.	3.1	46
121	ReaxFF reactive molecular dynamics on silicon pentaerythritol tetranitrate crystal validates the mechanism for the colossal sensitivity. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23779-23791.	2.8	21
122	Towards the rational design of polymers using molecular simulation: Predicting the effect of cure schedule on thermo-mechanical properties for a cycloaliphatic amine-cured epoxy resin. <i>Reactive and Functional Polymers</i> , 2014, 74, 1-15.	4.1	14
123	Adaptive Accelerated ReaxFF Reactive Dynamics with Validation from Simulating Hydrogen Combustion. <i>Journal of the American Chemical Society</i> , 2014, 136, 9434-9442.	13.7	53
124	Partially hydrogenated and fluorinated graphene: Structure, roughness, and negative thermal expansion. <i>Physical Review B</i> , 2015, 92, .	3.2	6
125	Derivatization and diffusive motion of molecular fullerenes: <i>Ab initio</i> and atomistic simulations. <i>Journal of Applied Physics</i> , 2015, 118, .	2.5	2
126	The transformation of silicon species contained in used oils under industrially relevant alkali treatment conditions. <i>Journal of Chemical Technology and Biotechnology</i> , 2015, 90, 1991-1998.	3.2	0
127	ReaxFF Reactive Molecular Dynamics Simulation of Functionalized Poly(phenylene oxide) Anion Exchange Membrane. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27727-27736.	3.1	68
128	Atomic-scale insight into the interactions between hydroxyl radicals and DNA in solution using the ReaxFF reactive force field. <i>New Journal of Physics</i> , 2015, 17, 103005.	2.9	37
129	Tribochemical Mechanism of Amorphous Silica Asperities in Aqueous Environment: A Reactive Molecular Dynamics Study. <i>Langmuir</i> , 2015, 31, 1429-1436.	3.5	54

#	ARTICLE	IF	CITATIONS
130	Effect of Fluence and Pulse Overlapping on Fabrication of Microchannels in PMMA/PDMS Via UV Laser Micromachining: Modeling and Experimentation. <i>Materials and Manufacturing Processes</i> , 2015, 30, 890-901.	4.7	25
131	A ReaxFF-based molecular dynamics study of the pyrolysis mechanism of polyimide. <i>Polymer Degradation and Stability</i> , 2015, 114, 72-80.	5.8	92
132	A ReaxFF Molecular Dynamics Study of the Pyrolysis Mechanism of Oleic-type Triglycerides. <i>Energy & Fuels</i> , 2015, 29, 5056-5068.	5.1	52
133	Microscopic study of the equation of state of \hat{I}^2 -HMX using reactive molecular dynamics simulations. <i>RSC Advances</i> , 2015, 5, 55892-55900.	3.6	3
134	Initial Pyrolysis Mechanism of Oil Shale Kerogen with Reactive Molecular Dynamics Simulation. <i>Energy & Fuels</i> , 2015, 29, 2987-2997.	5.1	58
135	The mechanisms for desensitization effect of synthetic polymers on BCHMX: Physical models and decomposition pathways. <i>Journal of Hazardous Materials</i> , 2015, 294, 145-157.	12.4	10
136	Doped polymer for low-loss dielectric material in the terahertz range. <i>Optical Materials Express</i> , 2015, 5, 1373.	3.0	26
137	Capturing material toughness by molecular simulation: accounting for large yielding effects and limits. <i>International Journal of Fracture</i> , 2015, 194, 149-167.	2.2	26
138	The effect of time step, thermostat, and strain rate on ReaxFF simulations of mechanical failure in diamond, graphene, and carbon nanotube. <i>Journal of Computational Chemistry</i> , 2015, 36, 1587-1596.	3.3	81
139	Chemisorption and thermally induced transformations of polydimethylsiloxane on the surface of nanoscale silica and ceria/silica. <i>Polymer Degradation and Stability</i> , 2015, 120, 203-211.	5.8	19
140	First principles-based multiparadigm, multiscale strategy for simulating complex materials processes with applications to amorphous SiC films. <i>Journal of Chemical Physics</i> , 2015, 142, 174703.	3.0	10
141	Reactive modeling of the initial stages of alkoxy silane polycondensation: effects of precursor molecule structure and solution composition. <i>Soft Matter</i> , 2015, 11, 6780-6789.	2.7	19
142	Simulation of the Elastic and Ultimate Tensile Properties of Diamond, Graphene, Carbon Nanotubes, and Amorphous Carbon Using a Revised ReaxFF Parametrization. <i>Journal of Physical Chemistry A</i> , 2015, 119, 9710-9721.	2.5	97
143	Environmental Chemistry of Organosiloxanes. <i>Chemical Reviews</i> , 2015, 115, 466-524.	47.7	231
144	The base-catalyzed transformation of tetramethyldisiloxane: influence of reaction media. <i>Journal of Chemical Technology and Biotechnology</i> , 2015, 90, 34-43.	3.2	3
145	Molecular-Level Modeling and Simulation in Process Safety. , 2016, , 111-210.		2
146	Photothermal Effects and Applications of Polydimethylsiloxane Membranes with Carbon Nanoparticles. <i>Polymers</i> , 2016, 8, 84.	4.5	28
147	Pyrolysis of CL20-BTF Co-crystal via ReaxFF-Ig Reactive Force Field Molecular Dynamics Simulations. <i>Chinese Journal of Chemical Physics</i> , 2016, 29, 557-563.	1.3	6

#	ARTICLE	IF	CITATIONS
148	Tailoring the mass distribution and functional group density of dimethylsiloxane-based films by thermal evaporation. <i>APL Materials</i> , 2016, 4, .	5.1	8
149	Research on Kapton aerobic pyrolysis by using ReaxFF molecular dynamics simulation. , 2016, , .		2
150	ReaxFF⁺â€”A New Reactive Force Field Method for the Accurate Description of Ionic Systems and Its Application to the Hydrolyzation of Aluminosilicates. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10849-10856.	3.1	8
151	Atomistic modeling framework for a cyclobutane-based mechanophore-embedded nanocomposite for damage precursor detection. <i>Computational Materials Science</i> , 2016, 120, 135-141.	3.0	9
152	Early and transient stages of Cu oxidation: Atomistic insights from theoretical simulations and in situ experiments. <i>Surface Science</i> , 2016, 652, 98-113.	1.9	37
153	Molecular dynamics study of brittle fracture in epoxy-based thermoset polymer. <i>Composites Part B: Engineering</i> , 2016, 95, 433-439.	12.0	51
154	Flexible, eco-friendly and highly sensitive paper antenna based electromechanical sensor for wireless human motion detection and structural health monitoring. <i>Extreme Mechanics Letters</i> , 2016, 9, 324-330.	4.1	40
155	Parameterization of the ReaxFF reactive force field for a proline-catalyzed aldol reaction. <i>Journal of Computational Chemistry</i> , 2016, 37, 2564-2572.	3.3	12
156	Degradation of polyacrylic elastomers: Theoretical and experimental studies. <i>Polymer Degradation and Stability</i> , 2016, 134, 60-75.	5.8	21
157	Theoretical Modeling of Thermal Decomposition of Methylnaphthalene Derivatives: Influence of Substituents. <i>Energy & Fuels</i> , 2016, 30, 6817-6821.	5.1	8
158	Molecular Dynamics Simulations Study of Brown Coal Pyrolysis Using ReaxFF Method. , 2016, , 59-67.		2
159	Atomistic Simulation of Solâ€”Gel-Derived Hybrid Materials. , 2016, , 1-34.		0
160	Water Interactions with Nanoporous Silica: Comparison of ReaxFF and <i>ab Initio</i> based Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24803-24816.	3.1	94
161	The fracture mechanism and the corresponding optimization strategy for nonhydrogenated amorphous carbon film in dimethyl silicone oil. <i>Surface and Coatings Technology</i> , 2016, 307, 941-950.	4.8	2
162	Hot spot formation and chemical reaction initiation in shocked HMX crystals with nanovoids: a large-scale reactive molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17627-17645.	2.8	52
163	Influence of density and environmental factors on decomposition kinetics of amorphous polylactide â€” Reactive molecular dynamics studies. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 67, 54-61.	2.4	13
164	Molecular dynamics simulations of nanoporous organosilicate glasses using Reactive Force Field (ReaxFF). <i>Journal of Non-Crystalline Solids</i> , 2016, 431, 103-111.	3.1	30
165	Accessing the free energy profile of a ring closure in a proline-catalyzed reaction using a reactive force field. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	4

#	ARTICLE	IF	CITATIONS
166	Development, applications and challenges of ReaxFF reactive force field in molecular simulations. <i>Frontiers of Chemical Science and Engineering</i> , 2016, 10, 16-38.	4.4	97
167	Reactive Molecular Dynamics on Massively Parallel Heterogeneous Architectures. <i>IEEE Transactions on Parallel and Distributed Systems</i> , 2017, 28, 202-214.	5.6	13
168	High fidelity and multi-scale thermal response modeling of an Avcoat-like TPS. , 2017, , .		2
169	Reactive molecular dynamics study of thermal decomposition of nanocarbon energetic composite materials. <i>Computational Materials Science</i> , 2017, 131, 126-131.	3.0	11
170	High-Temperature and High-Pressure Pyrolysis of Hexadecane: Molecular Dynamic Simulation Based on Reactive Force Field (ReaxFF). <i>Journal of Physical Chemistry A</i> , 2017, 121, 2069-2078.	2.5	44
171	High Toughness in Ultralow Density Graphene Oxide Foam. <i>Advanced Materials Interfaces</i> , 2017, 4, 1700030.	3.7	20
172	High-temperature pyrolysis simulation of acrylonitrile-butadiene model compound with experimental evidence. <i>Journal of Analytical and Applied Pyrolysis</i> , 2017, 125, 243-257.	5.5	16
173	Confinement effects on the thermal stability of poly(ethylene oxide)/graphene nanocomposites: A reactive molecular dynamics simulation study. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2017, 55, 1026-1035.	2.1	16
174	Reactive molecular dynamics simulations on the thermal decomposition of poly alpha-methyl styrene. <i>Journal of Molecular Modeling</i> , 2017, 23, 179.	1.8	8
175	Second-Generation ReaxFF Water Force Field: Improvements in the Description of Water Density and OH-Anion Diffusion. <i>Journal of Physical Chemistry B</i> , 2017, 121, 6021-6032.	2.6	87
176	Reactive force field simulation on thermal conductivities of carbon nanotubes and graphene. <i>International Journal of Heat and Mass Transfer</i> , 2017, 112, 903-912.	4.8	37
177	Time-Resolved Plasmonics used to Online Monitor Metal/Elastomer Deposition for Low-Voltage Dielectric Elastomer Transducers. <i>Advanced Electronic Materials</i> , 2017, 3, 1700073.	5.1	6
178	ReaxFF molecular dynamics simulation of pyrolysis and combustion of pyridine. <i>Fuel Processing Technology</i> , 2017, 161, 107-115.	7.2	72
179	Reactive molecular dynamics: an effective tool for modelling the sol-gel synthesis of bioglasses. <i>Journal of Materials Science</i> , 2017, 52, 9006-9013.	3.7	25
180	Dimeric anthracene-based mechanophore for damage precursor detection in epoxy-based thermoset polymer matrix: Characterization and atomistic modeling. <i>Computational Materials Science</i> , 2017, 133, 167-174.	3.0	12
181	Reactive Molecular Dynamics Simulation of Kerogen Thermal Maturation and Cross-Linking Pathways. <i>Energy & Fuels</i> , 2017, 31, 11601-11614.	5.1	28
182	Atomic-Level Simulation Study of n-Hexane Pyrolysis on Silicon Carbide Surfaces. <i>Langmuir</i> , 2017, 33, 11102-11108.	3.5	6
183	Thermal decomposition of HFO-1234yf through ReaxFF molecular dynamics simulation. <i>Applied Thermal Engineering</i> , 2017, 126, 330-338.	6.0	55

#	ARTICLE	IF	CITATIONS
184	Site Dependent Atom Type ReaxFF for the Proton-Catalyzed Twin Polymerization. <i>Journal of Physical Chemistry C</i> , 2017, 121, 15984-15992.	3.1	8
185	Lightweight Hexagonal Boron Nitride Foam for CO ₂ Absorption. <i>ACS Nano</i> , 2017, 11, 8944-8952.	14.6	56
186	Studies on the thermal properties of silicone polymer based thermal protection systems for space applications. <i>Journal of Thermal Analysis and Calorimetry</i> , 2017, 128, 1731-1741.	3.6	12
187	Effect of water content on the thermal degradation of amorphous polyamide 6,6: A collective variable-driven hyperdynamics study. <i>Polymer Degradation and Stability</i> , 2017, 146, 260-266.	5.8	18
188	High-temperature decomposition of the cellulose molecule: a stochastic molecular dynamics study. <i>Cellulose</i> , 2017, 24, 2713-2725.	4.9	63
189	Generation of amorphous carbon models using liquid quench method: A reactive molecular dynamics study. <i>Carbon</i> , 2017, 113, 87-99.	10.3	74
190	Validation of the COMPASS force field for complex inorganic-organic hybrid polymers. <i>Journal of Sol-Gel Science and Technology</i> , 2017, 81, 195-204.	2.4	31
191	Investigate the complex process in particle-fluid based surface generation technology using reactive molecular dynamics method. <i>AIP Advances</i> , 2017, 7, 075202.	1.3	0
192	Theoretical Study on Decomposition Mechanism of Insulating Epoxy Resin Cured by Anhydride. <i>Polymers</i> , 2017, 9, 341.	4.5	38
193	A Review of Multiscale Computational Methods in Polymeric Materials. <i>Polymers</i> , 2017, 9, 16.	4.5	138
194	Modeling the structure formation process of twin polymerization. <i>Reaction Kinetics, Mechanisms and Catalysis</i> , 2018, 123, 367-383.	1.7	5
195	Unexpected Rheology of Polydimethylsiloxane Liquid Blends. <i>Macromolecular Chemistry and Physics</i> , 2018, 219, 1700623.	2.2	4
196	Reactive Dynamics Simulation Study on the Pyrolysis of Polymer Precursors To Generate Amorphous Silicon Oxycarbide Structures. <i>Journal of Physical Chemistry C</i> , 2018, 122, 5767-5773.	3.1	17
197	CNTs-added PMNT/PDMS flexible piezoelectric nanocomposite for energy harvesting application. <i>Integrated Ferroelectrics</i> , 2018, 187, 70-79.	0.7	9
198	Bulk Polymer-Derived Ceramic Composites of Graphene Oxide. <i>ACS Omega</i> , 2018, 3, 4006-4016.	3.5	31
199	Micro-cracks on crosslinked Poly(dimethylsiloxane) (PDMS) surface treated by nanosecond laser irradiation. <i>Applied Surface Science</i> , 2018, 445, 488-495.	6.1	10
200	Initiation mechanisms and kinetic analysis of the isothermal decomposition of poly(<i>l</i> -methylstyrene): a ReaxFF molecular dynamics study. <i>RSC Advances</i> , 2018, 8, 3423-3432.	3.6	13
201	Si doping enhances the thermal stability of diamond-like carbon through reductions in carbon-carbon bond length disorder. <i>Carbon</i> , 2018, 131, 72-78.	10.3	59

#	ARTICLE	IF	CITATIONS
202	A ReaxFF-Based Molecular Dynamics Simulation of the Pyrolysis Mechanism for Polycarbonate. Energy & Fuels, 2018, 32, 2156-2162.	5.1	62
203	Mechanical Properties of Ultralow Density Graphene Oxide/Polydimethylsiloxane Foams. MRS Advances, 2018, 3, 61-66.	0.9	2
204	Reactive molecular dynamics simulation for analysis of thermal decomposition of oligomeric polyacrylic ester model nanocomposite and its experimental verification. Polymer, 2018, 137, 38-53.	3.8	24
205	Predicted detonation properties at the Chapman-Jouguet state for proposed energetic materials (MTO) Tj ETQq1 1 0.784314 rgBT Chemical Physics, 2018, 20, 3953-3969.	2.8	21
206	Network approach towards understanding the crazing in glassy amorphous polymers. Journal of Statistical Mechanics: Theory and Experiment, 2018, 2018, 043305.	2.3	2
207	3. Structure and Theory. , 2018, , 51-166.		0
208	Reactive Molecular Dynamics Study of Effects of Small-Molecule Organic Acids on PMIA Thermal Decomposition. Journal of Physical Chemistry B, 2018, 122, 10384-10392.	2.6	10
209	Atomistic mechanisms for chemical defects formation in polyethylene. Journal of Chemical Physics, 2018, 149, 234902.	3.0	11
210	Chemical Degradation Pathways in Siloxane Polymers Following Phenyl Excitations. Journal of Physical Chemistry B, 2018, 122, 12201-12210.	2.6	25
211	Designing reliable silicone elastomers for high-temperature applications. Polymer Degradation and Stability, 2018, 157, 175-180.	5.8	17
212	The role of hydrogen bonding in interaction energy at the interface of conductive polymers and modified graphene-based nanosheets: A reactive molecular dynamics study. Computational Materials Science, 2018, 155, 499-523.	3.0	13
213	Modeling Amorphous Microporous Polymers for CO ₂ Capture and Separations. Chemical Reviews, 2018, 118, 5488-5538.	47.7	208
214	Sustainable development of selective iron carbide, silicon carbide and ferrosilicon (low temperature) phases during iron ore reduction using only polymers. Sustainable Materials and Technologies, 2018, 16, 23-37.	3.3	6
215	Accelerated ReaxFF Simulations for Describing the Reactive Cross-Linking of Polymers. Journal of Physical Chemistry A, 2018, 122, 6633-6642.	2.5	96
216	The influence of oxygen on thermal decomposition characteristics of epoxy resins cured by anhydride. Polymer Degradation and Stability, 2018, 156, 125-131.	5.8	23
217	Underwater adhesive using solid-liquid polymer mixes. Materials Today Chemistry, 2018, 9, 149-157.	3.5	25
218	Dimethyl Ether Conversion into Light Olefins in a Slurry Reactor: Entrainment and Decomposition of Dispersion Liquid. Kinetics and Catalysis, 2019, 60, 681-687.	1.0	2
219	Mechanism and effect of thermal degradation on electrolyte ionic diffusivity in Li-ion batteries: A molecular dynamics study. Electrochimica Acta, 2019, 323, 134791.	5.2	21

#	ARTICLE	IF	CITATIONS
220	Partial CO ₂ Reduction in Amorphous Cylindrical Silica Nanopores Studied with Reactive Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 26358-26369.	3.1	4
221	Anisotropic Hydrolysis Susceptibility in Deformed Polydimethylsiloxanes. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7926-7935.	2.6	7
222	From ultra-high molecular weight polydimethylsiloxane to super-soft elastomer. <i>European Polymer Journal</i> , 2019, 120, 109243.	5.4	13
223	Effect of Ambient Chemistry on Friction at the Basal Plane of Graphite. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 40800-40807.	8.0	10
224	Modeling of PEM Fuel Cell Catalyst Layers: Status and Outlook. <i>Electrochemical Energy Reviews</i> , 2019, 2, 428-466.	25.5	60
225	Reactivity of Different Crystalline Surfaces of C3S During Early Hydration by the Atomistic Approach. <i>Materials</i> , 2019, 12, 1514.	2.9	11
226	The Constructions and Pyrolysis of 3D Kerogen Macromolecular Models: Experiments and Simulations. <i>Global Challenges</i> , 2019, 3, 1900006.	3.6	31
227	A reactive force field molecular dynamics study of molecular nitrogen and water mixtures under high temperature and high pressure. <i>Journal of Molecular Modeling</i> , 2019, 25, 120.	1.8	3
228	INFLUENCE OF NANOFILLER ON THERMAL DEGRADATION RESISTANCE OF HYDROGENATED NITRILE BUTADIENE RUBBER. <i>Rubber Chemistry and Technology</i> , 2019, 92, 263-285.	1.2	15
229	ReaxFF MD Simulations of Peptide-Grafted Gold Nanoparticles. <i>Langmuir</i> , 2019, 35, 5029-5036.	3.5	21
230	Influence of layered nanofillers on the mechanical properties and thermal degradation of polyacrylic ester polymer: Theoretical and experimental investigations. <i>Composites Part B: Engineering</i> , 2019, 169, 65-78.	12.0	24
231	Extracting the mechanisms and kinetic models of complex reactions from atomistic simulation data. <i>Journal of Computational Chemistry</i> , 2019, 40, 1586-1592.	3.3	20
232	Force Matching Approaches to Extend Density Functional Theory to Large Time and Length Scales. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 71-93.	0.6	5
233	Highly Stable Organic Transistors on Paper Enabled by a Simple and Universal Surface Planarization Method. <i>Advanced Materials Interfaces</i> , 2019, 6, 1801731.	3.7	10
234	Hydroxide transport and chemical degradation in anion exchange membranes: a combined reactive and non-reactive molecular simulation study. <i>Journal of Materials Chemistry A</i> , 2019, 7, 5442-5452.	10.3	39
235	Reactive molecular dynamics simulation of the thermal decomposition mechanisms of 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo[5.5.0.0.05,9.03,11]dodecane-4,10-dione (TEX). <i>Combustion and Flame</i> , 2019, 202, 303-317.	5.2	24
236	Multiscale Simulation on Product Distribution from Pyrolysis of Styrene-Butadiene Rubber. <i>Polymers</i> , 2019, 11, 1967.	4.5	13
237	Study on the thermal decomposition mechanism of graphene oxide functionalized with triaminoguanidine (GO-TAG) by molecular reactive dynamics and experiments. <i>RSC Advances</i> , 2019, 9, 33268-33281.	3.6	12

#	ARTICLE	IF	CITATIONS
238	First-principles ^{ab} -based reaction kinetics from reactive molecular dynamics simulations: Application to hydrogen peroxide decomposition. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18202-18208.	7.1	29
239	Material selection for optimum design of MEMS pressure sensors. Microsystem Technologies, 2020, 26, 2751-2766.	2.0	23
240	ReaxFF molecular dynamics simulations on the structure and dynamics of electrolyte water systems at ambient temperature. Computational Materials Science, 2020, 172, 109349.	3.0	21
241	ReacNetGenerator: an automatic reaction network generator for reactive molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 683-691.	2.8	54
242	High-temperature degradation of butadiene-based model elastomers by reactive molecular dynamics simulation. Journal of Applied Polymer Science, 2020, 137, 48592.	2.6	6
243	Molecular dynamics investigation on the gasification of a coal particle in supercritical water. International Journal of Hydrogen Energy, 2020, 45, 4254-4267.	7.1	30
244	Effect of oxidation degree on the thermal properties of graphene oxide. Journal of Materials Research and Technology, 2020, 9, 13740-13748.	5.8	32
245	A DFT Study on the Cyclization-Mechanism during Process of Thermal Vacuum Degradation for Poly(dimethylsiloxanes). Polymer Degradation and Stability, 2020, 182, 109367.	5.8	7
246	Investigation of iron carbide (Fe ₃ C) corrosion in water and acidic solution using ReaxFF molecular dynamics. Journal of Molecular Liquids, 2020, 318, 114006.	4.9	6
247	ReaxFF/AMBER: A Framework for Hybrid Reactive/Nonreactive Force Field Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7645-7654.	5.3	19
248	Atomistic-Scale Simulations of the Graphene Growth on a Silicon Carbide Substrate Using Thermal Decomposition and Chemical Vapor Deposition. Chemistry of Materials, 2020, 32, 8306-8317.	6.7	27
249	Material identification for improving the strength of silica/SBR interface using MD simulations. Journal of Molecular Modeling, 2020, 26, 234.	1.8	5
250	Reactive molecular dynamics research on influences of water on aging characteristics of PMIA insulation paper. Journal of Applied Physics, 2020, 127, 105107.	2.5	4
251	ReaxFF molecular dynamics simulations of electrolyte-water systems at supercritical temperature. Journal of Chemical Physics, 2020, 152, 204502.	3.0	11
252	Identifying Physical and Chemical Contributions to Friction: A Comparative Study of Chemically Inert and Active Graphene Step Edges. ACS Applied Materials & Interfaces, 2020, 12, 30007-30015.	8.0	6
253	Discovery and design of soft polymeric bio-inspired materials with multiscale simulations and artificial intelligence. Journal of Materials Chemistry B, 2020, 8, 6562-6587.	5.8	44
254	Benchmarking the Performance of the ReaxFF Reactive Force Field on Hydrogen Combustion Systems. Journal of Physical Chemistry A, 2020, 124, 5631-5645.	2.5	28
255	Thermal behavior study and degradation mechanism by TG/MS/FTIR technique of some poly(aryl ether) Tj ETQq1 1 0.784314 ggBT /Overl 5.5 19	5.5	19

#	ARTICLE	IF	CITATIONS
256	Impact of oxidation morphology on reduced graphene oxides upon thermal annealing. <i>JPhys Materials</i> , 2020, 3, 015011.	4.2	14
257	Silicone-epoxy block hybrid network to achieve high-performance and transparent polydimethylsiloxane materials. <i>Reactive and Functional Polymers</i> , 2020, 150, 104537.	4.1	16
258	Thermal decomposition of vegetable insulating oils from reactive molecular dynamics. <i>Chemical Physics Letters</i> , 2020, 746, 137284.	2.6	4
259	Polymerization Effects on the Decomposition of a Pyrazolo-Triazine at high Temperatures and Pressures. <i>ChemistryOpen</i> , 2020, 9, 470-479.	1.9	2
260	Molecular investigation on the compatibility of epoxy resin with liquid oxygen. <i>Theoretical and Applied Mechanics Letters</i> , 2020, 10, 38-45.	2.8	7
261	Molecular dynamics simulation of thermal degradation of silicone grease using reactive force field. <i>Journal of Applied Polymer Science</i> , 2021, 138, 50203.	2.6	3
262	Plasma polymerization of hexamethyldisiloxane: Revisited. <i>Plasma Processes and Polymers</i> , 2021, 18, 2000176.	3.0	36
263	Characterisation of pyrolysis kinetics and detailed gas species formations of engineering polymers via reactive molecular dynamics (ReaxFF). <i>Journal of Analytical and Applied Pyrolysis</i> , 2021, 153, 104931.	5.5	26
264	A Quantum-Based Approach to Predict Primary Radiation Damage in Polymeric Networks. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 463-473.	5.3	8
265	Origin of High Friction at Graphene Step Edges on Graphite. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 1895-1902.	8.0	16
266	Nanoscale modelling of polymer electrolytes for rechargeable batteries. <i>Energy Storage Materials</i> , 2021, 36, 77-90.	18.0	14
267	Atomic-scale insight into the pyrolysis of polycarbonate by ReaxFF-based reactive molecular dynamics simulation. <i>Fuel</i> , 2021, 287, 119484.	6.4	65
268	Effect of diol isomer/water mixtures on the stability of Zn-MOF-74. <i>Dalton Transactions</i> , 2021, 50, 1808-1815.	3.3	3
269	The initial reaction mechanism and thermal sensitivity of a fluoropolymer-containing energetic molecular system: the coupling effect of interfacial interactions and free radical reactions. <i>CrystEngComm</i> , 2021, 23, 3006-3014.	2.6	2
270	RMD simulations of ADN and ADN/GAP-based propellant. <i>Journal of the Brazilian Society of Mechanical Sciences and Engineering</i> , 2021, 43, 1.	1.6	5
271	In situ construction of fiber-supported micro-porous char structure to enhance anti-ablative performance of silicone rubber composites. <i>Polymers for Advanced Technologies</i> , 2021, 32, 2899-2907.	3.2	6
272	Additive manufacturing of structural materials. <i>Materials Science and Engineering Reports</i> , 2021, 145, 100596.	31.8	254
273	Evaluating the fire risk associated with cladding panels: An overview of fire incidents, policies, and future perspective in fire standards. <i>Fire and Materials</i> , 2021, 45, 663-689.	2.0	27

#	ARTICLE	IF	CITATIONS
274	Polymer informatics: Current status and critical next steps. <i>Materials Science and Engineering Reports</i> , 2021, 144, 100595.	31.8	117
275	Molecular Dynamics Simulation of Pyrolysis and Electric-caused Disintegration Mechanism of Polyphenylene Sulfide. , 2021, , .		0
277	Molecular dynamics simulation for investigating and assessing reaction conditions between carboxylated polyethersulfone and polyethyleneimine. <i>Journal of Applied Polymer Science</i> , 2021, 138, 51304.	2.6	1
278	3D Printable, Recyclable and Adjustable Comb/Bottlebrush Phase Change Polysiloxane Networks toward Sustainable Thermal Energy Storage. <i>Energy Storage Materials</i> , 2021, 39, 294-304.	18.0	43
279	Gamma Radiation Chemistry of Polydimethylsiloxane Foam in Radiation-Thermal Environments: Experiments and Simulations. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 41287-41302.	8.0	15
280	Elucidating multiple-scale reaction behaviors of phenolic resin pyrolysis via TG-FTIR and ReaxFF molecular dynamics simulations. <i>Journal of Analytical and Applied Pyrolysis</i> , 2021, 157, 105222.	5.5	50
281	Interfacial Bonding Controls Friction in Diamond-Rock Contacts. <i>Journal of Physical Chemistry C</i> , 2021, 125, 18395-18408.	3.1	9
282	Review: materials and modelling for organic photovoltaic devices. <i>Polymer International</i> , 0, , .	3.1	6
283	Photomechanical Polymer Nanocomposites for Drug Delivery Devices. <i>Molecules</i> , 2021, 26, 5376.	3.8	5
284	Microscopic pyrolysis mechanism on the octyphenylsiloxane flame retarded polycarbonate by reactive molecular dynamics. <i>Journal of Analytical and Applied Pyrolysis</i> , 2021, 158, 105274.	5.5	20
285	Molecular Dynamics and Machine Learning in Catalysts. <i>Catalysts</i> , 2021, 11, 1129.	3.5	15
286	Molecular dynamics investigation on supercritical water oxidation of a coal particle. <i>Journal of Analytical and Applied Pyrolysis</i> , 2021, 159, 105291.	5.5	5
287	Investigation of mechanical properties and dispersion in silica/Styrene Butadiene Rubber (SBR) nanocomposites: A ReaxFF molecular dynamics study. <i>Computational Materials Science</i> , 2021, 200, 110751.	3.0	8
288	A Reaxff-Based Molecular Dynamics Study of the Pyrolysis Mechanism of Hexamethyldisiloxane. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
289	Hierarchical Nanomechanics of Collagen Fibrils: Atomistic and Molecular Modeling. , 2008, , 175-247.		5
290	Ab initio quantum chemical and ReaxFF-based study of the intramolecular iminium-enamine conversion in a proline-catalyzed reaction. <i>Highlights in Theoretical Chemistry</i> , 2014, , 205-215.	0.0	1
291	Decomposition and Energy-Enhancement Mechanism of the Energetic Binder Glycidyl Azide Polymer at Explosive Detonation Temperatures. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5542-5554.	2.5	14
292	Molecular Dynamic Study of a Pyrolysis Process of a Coal Particle in Different Environments. <i>Journal of Energy Resources Technology, Transactions of the ASME</i> , 2020, 142, .	2.3	5

#	ARTICLE	IF	CITATIONS
293	Modeling Dynamic Fracture Using Large-Scale Atomistic Simulations. , 2006, , 1-68.		5
294	Theoretical Mass Spectra of PE, PP, PS and PET Polymers by QMD Methods Using the Model Molecules. Journal of Surface Analysis (Online), 2010, 17, 2-14.	0.1	2
295	High-temperature Adhesion Promoter Based on (3-Glycidoxypropyl) Trimethoxysilane for Cu Paste. Bulletin of the Korean Chemical Society, 2014, 35, 3025-3029.	1.9	12
296	Relationship between Atomic Structure, Composition, and Dielectric Constant in Zrâ€“SiO2 Glasses. ACS Omega, 2021, 6, 28561-28568.	3.5	2
297	Computational Scale Linking in Biological Protein Materials. , 2010, , 491-531.		0
298	Multiscale Modeling of Biological Protein Materials â€“ Deformation and Failure. Challenges and Advances in Computational Chemistry and Physics, 2010, , 473-533.	0.6	0
300	Computational Approaches and Simulation. Springer Series in Materials Science, 2012, , 213-263.	0.6	0
301	Molecular Modeling of the Microstructure of Soft Materials. , 2013, , .		0
302	Atomistic Simulation of Solâ€“Gel-Derived Hybrid Materials. , 2018, , 1869-1902.		0
303	Degradation of siliconeâ€“based materials as a driving force for recyclability. Polymer International, 2022, 71, 521-531.	3.1	22
304	Comparative Studies on Thermal Decompositions of Dinitropyrazole-Based Energetic Materials. Molecules, 2021, 26, 7004.	3.8	7
305	Aluminized Enhanced Blast Explosive Based on Polysiloxane Binder. Propellants, Explosives, Pyrotechnics, 2022, 47, .	1.6	1
306	An Investigation towards Coupling Molecular Dynamics with Computational Fluid Dynamics for Modelling Polymer Pyrolysis. Molecules, 2022, 27, 292.	3.8	12
307	ReaxFF/lg molecular dynamics study on thermal decomposition mechanism of 1-methyl-2,4,5-trinitroimidazole. Computational and Theoretical Chemistry, 2022, 1209, 113594.	2.5	9
308	Thermal decomposition of phosphonium salicylate and phosphonium benzoate ionic liquids. Journal of Molecular Liquids, 2022, 352, 118700.	4.9	12
310	Thermal and Thermo-Oxidative Degradation of Rubbers: Some Recent Studies. Advances in Polymer Science, 2021, , 1.	0.8	1
311	Capturing Free-Radical Polymerization by Synergetic <i>Ab Initio</i> Calculations and Topological Reactive Molecular Dynamics. Macromolecules, 2022, 55, 1474-1486.	4.8	3
312	A ReaxFF molecular dynamics study of insulation paper modification by plasma ROS. Physics of Plasmas, 2022, 29, .	1.9	5

#	ARTICLE	IF	CITATIONS
313	ReaxFF MD study on the early stage co-pyrolysis of mixed PE/PP/PS plastic waste. <i>Journal of Fuel Chemistry and Technology</i> , 2022, 50, 346-356.	2.0	10
314	Review of Molecular Dynamics Simulations of Phosphonium Ionic Liquid Lubricants. <i>Tribology Letters</i> , 2022, 70, 1.	2.6	8
315	Influence of external electric field on polymerization of Fe (III) flocculant in water: A reactive molecular dynamics and experiment study. <i>Journal of Molecular Liquids</i> , 2022, 352, 118741.	4.9	0
316	Chemical kinetics of hexamethyldisiloxane pyrolysis: A ReaxFF molecular dynamics simulation study. <i>International Journal of Chemical Kinetics</i> , 2022, 54, 413-423.	1.6	3
317	Decomposition properties of two phase immersion cooling medium C6F12O: A computational study. <i>Chemical Physics Letters</i> , 2022, 794, 139505.	2.6	3
318	Atomistic insights into the pyrolysis of methyl ethyl ketone peroxide via ReaxFF molecular dynamics simulation. <i>Chemical Engineering Research and Design</i> , 2022, 161, 316-324.	5.6	9
319	A ReaxFF-based molecular dynamics study of the pyrolysis mechanism of hexamethyldisiloxane. <i>Journal of Molecular Liquids</i> , 2022, 356, 119026.	4.9	11
320	Increasing the surface hydrophobicity of silicone rubber by electron beam irradiation in the presence of a glycerol layer. <i>Applied Surface Science</i> , 2022, 591, 153097.	6.1	15
321	Reactive molecular dynamics simulations of thermal and shear-driven oligomerization. <i>Applied Surface Science</i> , 2022, 591, 153209.	6.1	11
322	Hydrolytic Degradation of Polylactic Acid Fibers as a Function of pH and Exposure Time. <i>Molecules</i> , 2021, 26, 7554.	3.8	25
323	Superhydrophobic Carbon Nanotube-Metal Rubber Composites for Emulsion Separation. <i>ACS Applied Nano Materials</i> , 2021, 4, 13643-13654.	5.0	5
324	Leaching and Reactivity at the Sodium Aluminosilicate Glass-Water Interface: Insights from a ReaxFF Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27170-27184.	3.1	21
325	<i>Ab initio</i> neural network MD simulation of thermal decomposition of a high energy material CL-20/TNT. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 11801-11811.	2.8	13
326	Assessing pyrolysis behavior of silicon-containing arylacetylene resin via experiments and ReaxFF MD simulations. <i>Journal of Analytical and Applied Pyrolysis</i> , 2022, 164, 105528.	5.5	23
327	Molecular Dynamics Study of the Photodegradation of Polymeric Chains. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4374-4380.	4.6	2
328	Unexpected core-shell char from polycarbonate/polyborosiloxane composites and its application in improving flame retardancy. <i>Chemical Engineering Journal</i> , 2022, 446, 136742.	12.7	27
329	Reactive Molecular Dynamics Study of Hygrothermal Degradation of Crosslinked Epoxy Polymers. <i>ACS Applied Polymer Materials</i> , 2022, 4, 4411-4423.	4.4	11
330	Shear-activated chemisorption and association of cyclic organic molecules. <i>Faraday Discussions</i> , 0, 241, 194-205.	3.2	4

#	ARTICLE	IF	CITATIONS
331	Theoretical and experimental investigations into the pyrolysis mechanisms of silicon-modified phenolic resin under high temperatures. <i>Carbon</i> , 2023, 201, 504-519.	10.3	17
332	Accelerated Diffusion Following Deprotection in Chemically Amplified Resists. <i>Journal of Physical Chemistry B</i> , 0, , .	2.6	3
333	A review of molecular dynamics simulation in studying surface generation mechanism in ultra-precision cutting. <i>International Journal of Advanced Manufacturing Technology</i> , 2022, 122, 1195-1231.	3.0	4
334	Molecular insight into pyrolysis processes via reactive force field molecular dynamics: A state-of-the-art review. <i>Journal of Analytical and Applied Pyrolysis</i> , 2022, 166, 105620.	5.5	19
335	Mechanical properties of thermo-oxidative aged silicone rubber thermally stabilized by titanium oxide based fillers. <i>Polymer Testing</i> , 2022, 115, 107726.	4.8	8
336	Molecular dynamics simulation of glass transition and thermal stability of novel silicone elastomer and its nanocomposites. <i>Materials Today Communications</i> , 2022, 33, 104517.	1.9	3
337	High-temperature decomposition chemistry of trimethylsiloxane surfactants, a potential Fluorine-free replacement for fire suppression. <i>Chemosphere</i> , 2022, 308, 136351.	8.2	3
338	Classical, Coarse-Grained, and Reactive Molecular Dynamics Simulations on Polymer Nanocomposites. <i>Multiscale Science and Engineering</i> , 2022, 4, 161-178.	1.7	8
339	Microscopic pyrolysis mechanism of tert-butyl hydroperoxide via ReaxFF molecular dynamics. <i>Journal of Analytical and Applied Pyrolysis</i> , 2022, 168, 105727.	5.5	2
340	Tunable mechanical properties of vulcanised styrene-butadiene rubber by regulating cross-linked molecular network structures. <i>Molecular Simulation</i> , 0, , 1-8.	2.0	0
341	Interfacial carbon fiber-matrix interactions in thermosetting composites volumetrically cured by electromagnetic fields. <i>Composites Part A: Applied Science and Manufacturing</i> , 2023, 164, 107276.	7.6	7
342	On the Evolution of Additive Manufacturing (3D/4D Printing) Technologies: Materials, Applications, and Challenges. <i>Polymers</i> , 2022, 14, 4698.	4.5	23
343	Hyperthermal erosion of thermal protection nanocomposites under atomic oxygen and N ₂ bombardment. <i>International Journal of Mechanical Sciences</i> , 2023, 240, 107910.	6.7	5
344	An Adaptation of the Hoshen-Kopelman Cluster Counting Algorithm for Honeycomb Networks. , 2015, 8, 363-388.		1
345	Thermal decomposition mechanism investigation of hyperbranched polyglycerols by TGA-FTIR-GC/MS techniques and ReaxFF reactive molecular dynamics simulations. <i>Biomass and Bioenergy</i> , 2023, 168, 106675.	5.7	5
346	Bifunctional role of PDMS membrane in designing humidity-tolerant H ₂ S chemiresistors with high selectivity. <i>Chemical Communications</i> , 2023, 59, 1689-1692.	4.1	3
347	Insight into pyrolysis behavior of silicone-phenolic hybrid aerogel through thermal kinetic analysis and ReaxFF MD simulations. <i>Chemical Engineering Journal</i> , 2023, 458, 141480.	12.7	14
348	Molecular dynamics study on thermal decomposition characteristics of synthetic ester oil. <i>Chemical Physics Letters</i> , 2023, 813, 140302.	2.6	3

#	ARTICLE	IF	CITATIONS
349	New findings related to carbothermal reduction of polysiloxane-derived ceramics. <i>Ceramics International</i> , 2023, 49, 10193-10197.	4.8	2
350	Effects of Ambient Temperature on Nanosecond Laser Micro-Drilling of Polydimethylsiloxane (PDMS). <i>Micromachines</i> , 2023, 14, 90.	2.9	0
351	Chemical Modification of Dimethylpolysiloxane for Enhancement of CO ₂ Binding Enthalpy. <i>Physical Chemistry Chemical Physics</i> , 0, , .	2.8	0
352	Siloxane Molecules: Nonlinear Elastic Behavior and Fracture Characteristics. <i>Macromolecules</i> , 2023, 56, 1303-1310.	4.8	1
353	The evolution of carbon fiber elements and their effects on fiber mechanical properties from molecular dynamics. <i>Computational Materials Science</i> , 2023, 220, 112029.	3.0	4
354	Mechanisms of chemical-reaction-induced tensile deformation of an Fe/Ni/Cr alloy revealed by reactive atomistic simulations. <i>RSC Advances</i> , 2023, 13, 6630-6636.	3.6	1
355	Understanding SiOC atomic structures via synchrotron X-ray and reactive force field potential studies. <i>Materials Today Chemistry</i> , 2023, 29, 101429.	3.5	0
356	Formation and growth kinetics of the initial amorphous oxide film on the aluminum melt: A ReaxFF molecular dynamics simulation. <i>Computational Materials Science</i> , 2023, 220, 112035.	3.0	3
357	Oxidation decomposition mechanism of hexamethyldisiloxane. <i>Journal of Molecular Liquids</i> , 2023, 375, 121362.	4.9	2
358	Study on surface of polydimethylsiloxane irradiated by laser with assistance of pre-strain and its regulation on cell alignment. <i>Journal of Micromechanics and Microengineering</i> , 2023, 33, 045004.	2.6	0
359	Machine learning quantitatively characterizes the deformation and destruction of explosive molecules. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 8692-8704.	2.8	0
360	Back-to-cyclic monomers: chemical recycling of silicone waste using a [polydentate ligand-potassium silanolate] complex. <i>Green Chemistry</i> , 2023, 25, 3869-3877.	9.0	2
361	Molecular Simulations in Macromolecular Science. <i>Chinese Journal of Polymer Science (English)</i> Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 26	3.8	6
362	Micromechanism Study on Deterioration Effect of Vegetable Oil and Mineral Oil on Insulating Paper by Molecular Dynamics. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2023, 30, 1460-1469.	2.9	0
363	Development of a Ni-Al reactive force field for Ni-based superalloy: revealing electrostatic effects on mechanical deformation. <i>Journal of Materials Research and Technology</i> , 2023, 24, 4454-4467.	5.8	0
364	Investigation of Polymer Aging Mechanisms Using Molecular Simulations: A Review. <i>Polymers</i> , 2023, 15, 1928.	4.5	9
367	Review on Improving the Performance of SiO ₂ Anodes for a Lithium-Ion Battery through Insertion of Heteroatoms: State of the Art and Outlook. <i>Energy & Fuels</i> , 2023, 37, 13563-13578.	5.1	2
368	Defect Engineering of Graphene for Dynamic Reliability. <i>Small</i> , 0, , .	10.0	0

#	ARTICLE	IF	CITATIONS
369	Pyrolysis behaviors of di-tert-butyl peroxide in gas and liquid phases: A ReaxFF molecular dynamics simulation. <i>Fuel</i> , 2023, 351, 128930.	6.4	1
370	Time-resolved <i>in operando</i> analysis of the pyrolysis of a PECVD-deposited siloxane polymer using a combined DRIFTS-MS system. <i>Molecular Systems Design and Engineering</i> , 0, , .	3.4	0
371	Synergistic Effects of Gamma Irradiation, Tensile Stress and Moisture on the Radiolysis of Silicone Foam. <i>Chinese Journal of Polymer Science (English Edition)</i> , 0, , .	3.8	0
372	Nondestructive 3D Imaging of Microscale Damage inside Polymers—Based on the Discovery of Self-Excited Fluorescence Effect Induced by Electrical Field. <i>Advanced Science</i> , 2023, 10, .	11.2	2
373	ReaxFF Simulation of Pyrolysis Behaviors of Polysiloxane Precursors with Different Carbon Content. <i>Chemistry of Materials</i> , 2023, 35, 3902-3910.	6.7	3
374	Free Vibration Analysis of a Tunable Micro-Fabrication Device Comprising Asymmetric L-Shaped Membranes. <i>Polymers</i> , 2023, 15, 2293.	4.5	0
375	PXLink: A simulation program of polymer crosslinking to study of polyamide membrane. <i>Computer Physics Communications</i> , 2023, 291, 108840.	7.5	2
376	Investigating the pyrolysis mechanisms of three archetypal ablative resins through pyrolysis experiments and ReaxFF MD simulations. <i>Materials Today Communications</i> , 2023, 36, 106683.	1.9	0
377	Preparation and characterization of red mud/liquid silicon rubber with good thermal stability and processability. <i>Journal of Applied Polymer Science</i> , 2023, 140, .	2.6	0
378	A comprehensive study of pyrolysis characteristics of silicone-modified phenolic aerogel matrix Nanocomposites: Kinetic Analysis, ReaxFF MD Simulations, and ANN prediction. <i>Chemical Engineering Journal</i> , 2023, 472, 145049.	12.7	3
379	Graphene oxide coated silicon carbide films under projectile impacts. <i>International Journal of Mechanical Sciences</i> , 2024, 261, 108662.	6.7	1
380	Unveiling the Potential of Colorless Polyimide-Derived Laser-Induced Graphene: A Novel Pathway for Advanced Sensor and Energy Harvester Performance. <i>Advanced Materials Interfaces</i> , 2023, 10, .	3.7	0
381	Turning nanopowder into nanomaterial: Effect of continuous SiC coating on mechanical properties of Si nanoparticle arrays. <i>Materialia</i> , 2023, 32, 101906.	2.7	0
382	Mechano-Chemical Properties and Tribological Performance of Thin Perfluoropolyether (PFPE) Lubricant Film under Environmental Contaminants. <i>Lubricants</i> , 2023, 11, 306.	2.9	0
383	A detailed reaction mechanism for hexamethyldisiloxane combustion via experiments and ReaxFF molecular dynamics simulations. <i>International Journal of Chemical Kinetics</i> , 2024, 56, 131-149.	1.6	0
384	Atomic-scale insights into the tribochemical wear of diamond on quartz surfaces. <i>Applied Surface Science</i> , 2023, 639, 158152.	6.1	2
385	High-temperature failure mechanism and lifetime assessment of silicone gel package insulation for high-power electronic devices based on pyrolysis kinetics. <i>IEEE Transactions on Industry Applications</i> , 2023, , 1-12.	4.9	0
386	Thermal stability and thermal decomposition mechanism of octamethyltrisiloxane (MDM): Combined experiment, ReaxFF-MD and DFT study. <i>Energy</i> , 2023, 284, 129289.	8.8	1

#	ARTICLE	IF	CITATIONS
387	A comparative theoretical and experimental investigation on thermal parameters and initial pyrolysis mechanism of methyl-phenyl-dimethoxy silane modified phenolic resin. <i>Polymer Degradation and Stability</i> , 2023, 218, 110596.	5.8	0
388	Comparison on the Pyrolysis Characteristics of PDMS, PIB, and NTO Based on ReaxFF. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 2023, , 1-1.	2.9	0
390	Comparing the Tribological Performance of Water-Based and Oil-Based Drilling Fluids in Diamond-Rock Contacts. <i>Tribology Letters</i> , 2024, 72, .	2.6	0
391	Thermal Oxidation Behavior and Mechanisms for Silicon-Containing Arylacetylene Resins: Experimental and Reactive Force Field Molecular Dynamics Simulations. <i>ACS Applied Polymer Materials</i> , 2024, 6, 1962-1972.	4.4	0
392	Sustainable production of carbon nanomaterials based on TPT backsheet pyrolysis from end-of-life photovoltaic modules. <i>Separation and Purification Technology</i> , 2024, 339, 126689.	7.9	0
393	Shear-activation of mechanochemical reactions through molecular deformation. <i>Scientific Reports</i> , 2024, 14, .	3.3	0
394	A multiscale modeling framework for predicting strain-dependent electrical conductivity of carbon nanotube-incorporated nanocomposites considering the electron tunneling effect. <i>Polymer Composites</i> , 0, , .	4.6	0
395	Experimental and Computational Studies on Surface Characteristics of Silica Particles Synthesized by Hexamethyldisiloxane Combustion. <i>Silicon</i> , 0, , .	3.3	0