Yue Qi

List of Publications by Year in descending order

148 papers	12,577 citations	30070 54 h-index	24982 109 g-index
151 all docs	151 docs citations	151 times ranked	11199 citing authors

#	Article	IF	Citations
1	Predicting low-impedance interfaces for solid-state batteries. Current Opinion in Solid State and Materials Science, 2022, 26, 100990.	11.5	9
2	Carbon-Nanotube-Encapsulated-Sulfur Cathodes for Lithiumâ€“Sulfur Batteries: Integrated Computational Design and Experimental Validation. Nano Letters, 2022, 22, 441-447.	9.1	12
3	A high-performance hydroxide exchange membrane enabled by Cu2+-crosslinked chitosan. Nature Nanotechnology, 2022, 17, 629-636.	31.5	50
4	Electrochemical Birch Reduction: A Molecular-Level Venture into the Solvation Structure at the Electrode Interface. ECS Meeting Abstracts, 2022, MA2022-01, 1966-1966.	0.0	0
5	Redox-couple investigations in Si-doped Li-rich cathode materials. Physical Chemistry Chemical Physics, 2021, 23, 2780-2791.	2.8	6
6	Dendrite-free Lithium Based on Lessons Learned from Lithium and Magnesium Electrodeposition Morphology Simulations. Cell Reports Physical Science, 2021, 2, 100294.	5.6	19
7	Modeling the electrical double layer at solid-state electrochemical interfaces. Nature Computational Science, 2021, 1, 212-220.	8.0	35
8	Patterned nickel interlayers for enhanced silver wetting, spreading and adhesion on ceramic substrates. Scripta Materialia, 2021, 196, 113767.	5.2	4
9	Maintaining a Flat Li Surface during the Li Stripping Process via Interface Design. Chemistry of Materials, 2021, 33, 2814-2823.	6.7	25
10	Interfacial toughening with self-assembled monolayers enhances perovskite solar cell reliability. Science, 2021, 372, 618-622.	12.6	313
11	Impact of Electronic Properties of Grain Boundaries on the Solid Electrolyte Interphases (SEIs) in Li-ion Batteries. Journal of Physical Chemistry C, 2021, 125, 15821-15829.	3.1	18
12	Copper-coordinated cellulose ion conductors for solid-state batteries. Nature, 2021, 598, 590-596.	27.8	262
13	Spatially Resolved Potential and Li-Ion Distributions Reveal Performance-Limiting Regions in Solid-State Batteries. ACS Energy Letters, 2021, 6, 3944-3951.	17.4	18
14	How Transition Metals Enable Electron Transfer through the SEI: Part I. Experiments and Butler-Volmer Modeling. Journal of the Electrochemical Society, 2020, 167, 013502.	2.9	17
15	Enhanced liquid metal wetting on oxide surfaces via patterned particles. Acta Materialia, 2020, 199, 551-560.	7.9	11
16	Optimization of the Reax force field for the lithiumâ€“oxygen system using a high fidelity charge model. Journal of Chemical Physics, 2020, 153, 084107.	3.0	11
17	A New General Paradigm for Understanding and Preventing Li Metal Penetration through Solid Electrolytes. Joule, 2020, 4, 2599-2608.	24.0	71
18	Wavelet scattering networks for atomistic systems with extrapolation of material properties. Journal of Chemical Physics, 2020, 153, 084109.	3.0	8

#	Article	IF	Citations
19	The Bonding Nature and Adhesion of Polyacrylic Acid Coating on Li-Metal for Li Dendrite Prevention. ACS Applied Materials & Interfaces, 2020, 12, 51007-51015.	8.0	21
20	Reversible planar gliding and microcracking in a single-crystalline Ni-rich cathode. Science, 2020, 370, 1313-1317.	12.6	472
21	Evaluation of The Electrochemo-Mechanically Induced Stress in All-Solid-State Li-Ion Batteries. Journal of the Electrochemical Society, 2020, 167, 090541.	2.9	43
22	Efficient Low-Temperature Cycling of Lithium Metal Anodes by Tailoring the Solid-Electrolyte Interphase. ACS Energy Letters, 2020, 5, 2411-2420.	17.4	174
23	Compositions and Formation Mechanisms of Solid-Electrolyte Interphase on Microporous Carbon/Sulfur Cathodes. Chemistry of Materials, 2020, 32, 3765-3775.	6.7	27
24	Composition, crystallography, and oxygen vacancy ordering impacts on the oxygen ion conductivity of lanthanum strontium ferrite. Physical Chemistry Chemical Physics, 2020, 22, 9723-9733.	2.8	10
25	The origin of the two-plateaued or one-plateaued open circuit voltage in Liâ€“S batteries. Nano Energy, 2020, 75, 104915.	16.0	28
26	Interfacial Electronic Properties Dictate Li Dendrite Growth in Solid Electrolytes. Chemistry of Materials, 2019, 31, 7351-7359.	6.7	165
27	Cathode porosity is a missing key parameter to optimize lithium-sulfur battery energy density. Nature Communications, 2019, 10, 4597.	12.8	166
28	Mechanical and Electronic Stabilization of Solid Electrolyte Interphase with Sulfite Additive for Lithium Metal Batteries. Journal of the Electrochemical Society, 2019, 166, A3201-A3206.	2.9	8
29	First-Principles Prediction of Potentials and Space-Charge Layers in All-Solid-State Batteries. Physical Review Letters, 2019, 122, 167701.	7.8	57
30	Energy landscape of the charge transfer reaction at the complex Li/SEI/electrolyte interface. Energy and Environmental Science, 2019, 12, 1286-1295.	30.8	85
31	Connecting Oxide Bifilmsâ€™ Properties from Atomistic Simulations with Virtual Casting of Aluminum. Minerals, Metals and Materials Series, 2019, , 45-51.	0.4	3
32	Highâ€Energy Rechargeable Metallic Lithium Battery at â^'70â€‰Â°C Enabled by a Cosolvent Electrolyte. Angewandte Chemie, 2019, 131, 5679-5683.	2.0	52
33	Highâ€Energy Rechargeable Metallic Lithium Battery at â^'70â€‰Â°C Enabled by a Cosolvent Electrolyte. Angewandte Chemie - International Edition, 2019, 58, 5623-5627.	13.8	217
34	Adsorption of Lignin Î²-O-4 Dimers on Metal Surfaces in Vacuum and Solvated Environments. ACS Sustainable Chemistry and Engineering, 2019, 7, 2667-2678.	6.7	11
35	Atomistic simulation of the formation and fracture of oxide bifilms in cast aluminum. Acta Materialia, 2019, 164, 673-682.	7.9	35
36	Computational design of metal oxides to enhance the wetting and adhesion of silver-based brazes on yttria-stabilized-zirconia. Acta Materialia, 2018, 152, 229-238.	7.9	39

#	Article	IF	Citations
37	From Microparticles to Nanowires and Back: Radical Transformations in Plated Li Metal Morphology Revealed via in Situ Scanning Electron Microscopy. Nano Letters, 2018, 18, 1644-1650.	9.1	47
38	Nanoscale Protection Layers To Mitigate Degradation in High-Energy Electrochemical Energy Storage Systems. Accounts of Chemical Research, 2018, 51, 97-106.	15.6	33
39	Transferable Self-Consistent Charge Density Functional Tight-Binding Parameters for Liâ€“Metal and Li-Ions in Inorganic Compounds and Organic Solvents. Journal of Physical Chemistry C, 2018, 122, 10755-10764.	3.1	22
40	Review on modeling of the anode solid electrolyte interphase (SEI) for lithium-ion batteries. Npj Computational Materials, 2018, 4, .	8.7	961
41	Si-doped high-energy Li_{1.2}Mn_{0.54}Ni_{0.13}Co_{0.13}O₂ cathode with improved capacity for lithium-ion batteries. Journal of Materials Research, 2018, 33, 4182-4191.	2.6	9
42	A Bottom-Up Formation Mechanism of Solid Electrolyte Interphase Revealed by Isotope-Assisted Time-of-Flight Secondary Ion Mass Spectrometry. Journal of Physical Chemistry Letters, 2018, 9, 5508-5514.	4.6	29
43	Anisotropic chemical strain in cubic ceria due to oxygen-vacancy-induced elastic dipoles. Physical Chemistry Chemical Physics, 2018, 20, 15293-15299.	2.8	24
44	Computational study of lithium nucleation tendency in Li7La3Zr2O12 (LLZO) and rational design of interlayer materials to prevent lithium dendrites. Journal of Power Sources, 2018, 392, 79-86.	7.8	144
45	Atomistic Origin of Deformation Twinning in Biomineral Aragonite. Physical Review Letters, 2017, 118, 105501.	7.8	25
46	Atomistic Simulation Derived Insight on the Irreversible Structural Changes of Si Electrode during Fast and Slow Delithiation. Nano Letters, 2017, 17, 4330-4338.	9.1	40
47	Long-range charge transfer and oxygen vacancy interactions in strontium ferrite. Journal of Materials Chemistry A, 2017, 5, 4493-4506.	10.3	69
48	Integrated Computation and Experimental Investigation on the Adsorption Mechanisms of Anti-Wear and Anti-Corrosion Additives on Copper. Journal of Physical Chemistry C, 2017, 121, 21995-22003.	3.1	8
49	In situ stress measurements during electrochemical cycling of lithium-rich cathodes. Journal of Power Sources, 2017, 364, 383-391.	7.8	18
50	Computationally Driven Two-Dimensional Materials Design: What Is Next?. ACS Nano, 2017, 11, 7560-7564.	14.6	39
51	First-Principles Studies of Oxygen Vacancy Interactions and Their Impact on Oxygen Migration in Lanthanum Strontium Ferrite. ECS Transactions, 2017, 78, 2807-2814.	0.5	5
52	Polaron size and shape effects on oxygen vacancy interactions in lanthanum strontium ferrite. Journal of Materials Chemistry A, 2017, 5, 25031-25043.	10.3	29
53	How Solid-Electrolyte Interphase Forms in Aqueous Electrolytes. Journal of the American Chemical Society, 2017, 139, 18670-18680.	13.7	365
54	Simulation of the Effect of Contact Area Loss in All-Solid-State Li-Ion Batteries. Journal of the Electrochemical Society, 2017, 164, E3512-E3521.	2.9	111

#	Article	IF	Citations
55	Atomic Insight into the Lithium Storage and Diffusion Mechanism of SiO₂/Al₂O₃ Electrodes of Lithium Ion Batteries: ReaxFF Reactive Force Field Modeling. Journal of Physical Chemistry A, 2016, 120, 2114-2127.	2.5	80
56	Computational Exploration of the Li-Electrode | Electrolyte Interface in the Presence of a Nanometer Thick Solid-Electrolyte Interphase Layer. Accounts of Chemical Research, 2016, 49, 2363-2370.	15.6	124
57	Ab initiodiffuse-interface model for lithiated electrode interface evolution. Physical Review E, 2016, 94, 012802.	2.1	7
58	Stabilizing high voltage LiCoO₂ cathode in aqueous electrolyte with interphase-forming additive. Energy and Environmental Science, 2016, 9, 3666-3673.	30.8	190
59	Computational Analysis of Coupled Anisotropic Chemical Expansion in Li2-XMnO3-Î´. MRS Advances, 2016, 1, 1037-1042.	0.9	4
60	Self-generated concentration and modulus gradient coating design to protect Si nano-wire electrodes during lithiation. Physical Chemistry Chemical Physics, 2016, 18, 3706-3715.	2.8	42
61	Interfacial Study on Solid Electrolyte Interphase at Li Metal Anode: Implication for Li Dendrite Growth. Journal of the Electrochemical Society, 2016, 163, A592-A598.	2.9	180
62	The impact of oxygen vacancies on lithium vacancy formation and diffusion in Li2-MnO3-. Solid State Ionics, 2016, 289, 87-94.	2.7	21
63	Design of Nanostructured Heterogeneous Solid Ionic Coatings through a Multiscale Defect Model. ACS Applied Materials & Interfaces, 2016, 8, 5687-5693.	8.0	53
64	Synergetic Effects of Inorganic Components in Solid Electrolyte Interphase on High Cycle Efficiency of Lithium Ion Batteries. Nano Letters, 2016, 16, 2011-2016.	9.1	320
65	Connecting the irreversible capacity loss in Li-ion batteries with the electronic insulating properties of solid electrolyte interphase (SEI) components. Journal of Power Sources, 2016, 309, 221-230.	7.8	182
66	Modulation of dendritic patterns during electrodeposition: A nonlinear phase-field model. Journal of Power Sources, 2015, 300, 376-385.	7.8	235
67	Dissecting graphene capacitance in electrochemical cell. Electrochimica Acta, 2015, 163, 296-302.	5.2	18
68	General method to predict voltage-dependent ionic conduction in a solid electrolyte coating on electrodes. Physical Review B, 2015, 91, .	3.2	141
69	Vacancies in Si Can Improve the Concentration-Dependent Lithiation Rate: Molecular Dynamics Studies of Lithiation Dynamics of Si Electrodes. Journal of Physical Chemistry C, 2015, 119, 24265-24275.	3.1	17
70	Lithium Concentration Dependent Elastic Properties of Battery Electrode Materials from First Principles Calculations. Journal of the Electrochemical Society, 2014, 161, F3010-F3018.	2.9	231
71	Understanding and Predicting the Lithium Dendrite Formation in Li-Ion Batteries: Phase Field Model. ECS Transactions, 2014, 61, 1-9.	0.5	13
72	Unveiling the environment-dependent mechanical properties of porous polypropylene separators. Polymer, 2014, 55, 6282-6292.	3.8	54

#	Article	IF	Citations
73	Introduction to Mechano-Electro-Chemical Coupling in Energy Related Materials and Devices. Journal of the Electrochemical Society, 2014, 161, Y11-Y12.	2.9	9
74	Deformation and fracture behaviors of microporous polymer separators for lithium ion batteries. RSC Advances, 2014, 4, 14904.	3.6	57
75	Property Evolution of Al₂O₃Coated and Uncoated Si Electrodes: A First Principles Investigation. Journal of the Electrochemical Society, 2014, 161, F3137-F3143.	2.9	36
76	From Ab Initio Calculations to Multiscale Design of Si/C Coreâ€“Shell Particles for Li-Ion Anodes. Nano Letters, 2014, 14, 2140-2149.	9.1	29
77	Oxidation-assisted ductility of aluminium nanowires. Nature Communications, 2014, 5, 3959.	12.8	66
78	Probing the Roles of Polymeric Separators in Lithium-Ion Battery Capacity Fade at Elevated Temperatures. Journal of the Electrochemical Society, 2014, 161, A1241-A1246.	2.9	30
79	On the La2/3â^'xLi3xTiO3/Al2O3 composite solid-electrolyte for Li-ion conduction. Journal of Alloys and Compounds, 2013, 577, 57-63.	5.5	35
80	Improving microstructure of silicon/carbon nanofiber composites as a Li battery anode. Journal of Power Sources, 2013, 221, 455-461.	7.8	50
81	Oxidation induced softening in Al nanowires. Applied Physics Letters, 2013, 102, .	3.3	36
82	Unveiling the Roles of Binder in the Mechanical Integrity of Electrodes for Lithium-Ion Batteries. Journal of the Electrochemical Society, 2013, 160, A1502-A1509.	2.9	139
83	Low friction and environmentally stable diamond-like carbon (DLC) coatings incorporating silicon, oxygen and fluorine sliding against aluminum. Surface and Coatings Technology, 2013, 215, 340-349.	4.8	38
84	A Beaded-String Silicon Anode. ACS Nano, 2013, 7, 2717-2724.	14.6	68
85	Defect Thermodynamics and Diffusion Mechanisms in Li₂CO₃ and Implications for the Solid Electrolyte Interphase in Li-Ion Batteries. Journal of Physical Chemistry C, 2013, 117, 8579-8593.	3.1	228
86	Li Segregation Induces Structure and Strength Changes at the Amorphous Si/Cu Interface. Nano Letters, 2013, 13, 4759-4768.	9.1	75
87	Stress Contributions to Solution Thermodynamics in Li-Si Alloys. Electrochemical and Solid-State Letters, 2012, 15, A9.	2.2	70
88	Publisher's Note: Stress Contributions to Solution Thermodynamics in Li-Si Alloys [Electrochem. Solid-State Lett., 15, A9 (2012)]. Electrochemical and Solid-State Letters, 2012, 15, S3.	2.2	5
89	Nonlinear phase-field model for electrode-electrolyte interface evolution. Physical Review E, 2012, 86, 051609.	2.1	100
90	Conductivity of an atomically defined metallic interface. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 19097-19102.	7.1	25

#	Article	IF	Citations
91	Chemically Induced Crack Instability When Electrodes Fracture. Journal of the Electrochemical Society, 2012, 159, A1838-A1843.	2.9	22
92	Visualizing the chemistry and structure dynamics in lithium-ion batteries by in-situ neutron diffraction. Scientific Reports, 2012, 2, 747.	3.3	134
93	Lattice dynamics, thermodynamics and elastic properties of monoclinic Li2CO3 from density functional theory. Acta Materialia, 2012, 60, 5204-5216.	7.9	64
94	Direct Calculation of Li-Ion Transport in the Solid Electrolyte Interphase. Journal of the American Chemical Society, 2012, 134, 15476-15487.	13.7	524
95	The Mixing Mechanism during Lithiation of Si Negative Electrode in Li-Ion Batteries: An Ab Initio Molecular Dynamics Study. Nano Letters, 2011, 11, 5494-5500.	9.1	155
96	Using Atomic Layer Deposition to Hinder Solvent Decomposition in Lithium Ion Batteries: First-Principles Modeling and Experimental Studies. Journal of the American Chemical Society, 2011, 133, 14741-14754.	13.7	174
97	Role of oxygen and humidity on the tribo-chemical behaviour of non-hydrogenated diamond-like carbon coatings. Wear, 2011, 271, 2157-2163.	3.1	59
98	The Effect of Solute Atoms on Aluminum Grain Boundary Sliding at Elevated Temperature. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2011, 42, 651-659.	2.2	28
99	Material transfer mechanisms between aluminum and fluorinated carbon interfaces. Acta Materialia, 2011, 59, 2601-2614.	7.9	49
100	Mesoscale modeling of the influence of morphology on the mechanical properties of proton exchange membranes. Polymer, 2011, 52, 201-210.	3.8	22
101	First-principles study of void induced stresses at a diamond (100) grain boundary. Journal of Applied Physics, 2011, 109, 033518.	2.5	6
102	Elastic softening of amorphous and crystalline Liâ€“Si Phases with increasing Li concentration: A first-principles study. Journal of Power Sources, 2010, 195, 6825-6830.	7.8	367
103	Aluminum Î£3 grain boundary sliding enhanced by vacancy diffusion. Acta Materialia, 2010, 58, 4245-4252.	7.9	21
104	Environmental conditions to achieve low adhesion and low friction on diamond surfaces. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 034008.	2.0	36
105	Mesopores inside electrode particles can change the Li-ion transport mechanism and diffusion-induced stress. Journal of Materials Research, 2010, 25, 1433-1440.	2.6	82
106	Adhesion at diamond/metal interfaces: A density functional theory study. Journal of Applied Physics, 2010, 107, .	2.5	46
107	Effects of Concentration-Dependent Elastic Modulus on Diffusion-Induced Stresses for Battery Applications. Journal of the Electrochemical Society, 2010, 157, A967.	2.9	145
108	Threefold Increase in the Youngâ€™s Modulus of Graphite Negative Electrode during Lithium Intercalation. Journal of the Electrochemical Society, 2010, 157, A558.	2.9	348

#	Article	IF	Citations
109	In Situ Observation of Strains during Lithiation of a Graphite Electrode. Journal of the Electrochemical Society, 2010, 157, A741.	2.9	205
110	Enhance diamond coating adhesion by oriented interlayer microcracking. Journal of Applied Physics, 2009, 106, 123514.	2.5	2
111	Surface stability and electronic structure of hydrogen- and fluorine-terminated diamond surfaces: A first-principles investigation. Journal of Materials Research, 2009, 24, 2461-2470.	2.6	38
112	Engineering size-scaling of plastic deformation in nanoscale asperities. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 9580-9585.	7.1	21
113	Phase transition and morphology of polydispersed ABAâ€² triblock copolymers determined by continuous and discrete simulations. Journal of Chemical Physics, 2009, 130, 064902.	3.0	12
114	The influence of heterogeneity in grain boundary sliding resistance on the constitutive behavior of AA5083 during high-temperature deformation. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2009, 504, 175-182.	5.6	9
115	Strength characterization of Al/Si interfaces: A hybrid method of nanoindentation and finite element analysis. Acta Materialia, 2009, 57, 695-707.	7.9	31
116	A molecular dynamics simulation study of hydrated sulfonated poly(ether ether ketone) for application to polymer electrolyte membrane fuel cells: Effect of water content. Journal of Renewable and Sustainable Energy, 2009, 1, .	2.0	51
117	Non-bonded force field for the interaction between metals and organic molecules: a case study of olefins on aluminum. Physical Chemistry Chemical Physics, 2009, 11, 10195.	2.8	14
118	Critical shear stresses at aluminumâ€“silicon interfaces. Acta Materialia, 2008, 56, 3461-3469.	7.9	35
119	Surface Stability and Electronic Structure of Hydrogen and Fluorine Terminated Diamond Surfaces: a First Principles Investigation. Materials Research Society Symposia Proceedings, 2008, 1130, 63001.	0.1	0
120	Predicting the hydrogen pressure to achieve ultralow friction at diamond and diamondlike carbon surfaces from first principles. Applied Physics Letters, 2008, 92, .	3.3	29
121	Intrinsic stress evolution in nanocrystalline diamond thin films with deposition temperature. Applied Physics Letters, 2008, 92, .	3.3	28
122	Origin of static friction and its relationship to adhesion at the atomic scale. Physical Review B, 2007, 75, .	3.2	30
123	Elucidating the contact mechanics of aluminum silicon surfaces with Green's function molecular dynamics. Journal of Applied Physics, 2007, 102, 113511.	2.5	8
124	Planar stacking effect on elastic stability of hexagonal boron nitride. Applied Physics Letters, 2007, 90, 081922.	3.3	38
125	Partial-mediated slips in nanocrystalline Ni at high strain rate. Applied Physics Letters, 2007, 90, 221911.	3.3	36
126	Ab initiostudy of the effect of solute atoms on the stacking fault energy in aluminum. Physical Review B, 2007, 75, .	3.2	94

#	Article	IF	Citations
127	Molecular dynamics simulations of grain boundary sliding: The effect of stress and boundary misorientation. Acta Materialia, 2007, 55, 1555-1563.	7.9	93
128	Mechanical behavior of aluminumâ€“silicon nanocomposites: A molecular dynamics study. Acta Materialia, 2006, 54, 4441-4451.	7.9	54
129	Aluminumâ€“silicon interfaces and nanocomposites: A molecular dynamics study. Composites Science and Technology, 2006, 66, 1151-1161.	7.8	44
130	Atmospheric effects on the adhesion and friction between non-hydrogenated diamond-like carbon (DLC) coating and aluminum â€“ A first principles investigation. Surface Science, 2006, 600, 2955-2965.	1.9	155
131	Mesoscale simulation of morphology in hydrated perfluorosulfonic acid membranes. Journal of Chemical Physics, 2006, 124, 134702.	3.0	168
132	A first principles study of adhesion and adhesive transfer at Al(111)/graphite(0001). Surface Science, 2005, 581, 155-168.	1.9	47
133	Atomic simulations of kinetic friction and its velocity dependence atAlâˆ•AlandÎ±â€²Al2O3âˆ•Î±â€²Al2O3interfaces. Physical Review B, 2005, 72, .	3.2	42
134	Adhesion and nonwetting-wetting transition in theAl/Î±â€²Al2O3interface. Physical Review B, 2004, 69, .	3.2	184
135	Adhesion and adhesive transfer at aluminum/diamond interfaces:â€,A first-principles study. Physical Review B, 2004, 69, .	3.2	118
136	Hydrogen effect on adhesion and adhesive transfer at aluminum/diamond interfaces. Physical Review B, 2003, 68, .	3.2	46
137	Friction anisotropy at Ni(100)/(100) interfaces:â€ƒMolecular dynamics studies. Physical Review B, 2002, 66, .	3.2	55
138	First principles multiscale modeling of physico-chemical aspects of tribology. Tribology Series, 2001, , 15-33.	0.1	1
139	Large scale atomistic simulations of screw dislocation structure, annihilation and cross-slip in FCC Ni. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2001, 309-310, 156-159.	5.6	24
140	MPiSIM: Massively parallel simulation tool for metallic system. Journal of Computer-Aided Materials Design, 2001, 8, 185-192.	0.7	2
141	Viscosities of liquid metal alloys from nonequilibrium molecular dynamics. Journal of Computer-Aided Materials Design, 2001, 8, 233-243.	0.7	79
142	Melting and crystallization in Ni nanoclusters: The mesoscale regime. Journal of Chemical Physics, 2001, 115, 385-394.	3.0	345
143	Molecular Dynamics Simulations of Supercooled Liquid Metals and Glasses. Materials Research Society Symposia Proceedings, 2000, 644, 231.	0.1	2
144	Molecular-dynamics simulations of glass formation and crystallization in binary liquid metals:â€ƒCu-Ag and Cu-Ni. Physical Review B, 1999, 59, 3527-3533.	3.2	252

#	Article	IF	Citations
145	Computational Materials Chemistry at the Nanoscale. Journal of Nanoparticle Research, 1999, 1, 51-69.	1.9	23
146	Strain Rate Induced Amorphization in Metallic Nanowires. Physical Review Letters, 1999, 82, 2900-2903.	7.8	268
147	Calculation of Mechanical, Thermodynamic and Transport Properties of Metallic Glass Formers. Materials Research Society Symposia Proceedings, 1998, 554, 43.	0.1	117
148	Deformation Behavior of FCC Crystalline Metallic Nanowires Under High Strain Rates. Materials Research Society Symposia Proceedings, 1998, 554, 367.	0.1	1