Yue Qi

List of Publications by Year in Descending Order

146 papers	8,913 citations	50 h-index	91 g-index
151 ext. papers	10,634 ext. citations	8.1 avg, IF	6.62 L-index

#	Paper	IF	Citations
146	Predicting low-impedance interfaces for solid-state batteries. *Current Opinion in Solid State and Materials Science*, **2022**, 26, 100990	12	1
145	Copper-coordinated cellulose ion conductors for solid-state batteries. *Nature*, **2021**, 598, 590-596	50.4	49
144	Patterned nickel interlayers for enhanced silver wetting, spreading and adhesion on ceramic substrates. *Scripta Materialia*, **2021**, 196, 113767	5.6	1
143	Maintaining a Flat Li Surface during the Li Stripping Process via Interface Design. *Chemistry of Materials*, **2021**, 33, 2814-2823	9.6	10
142	Interfacial toughening with self-assembled monolayers enhances perovskite solar cell reliability. *Science*, **2021**, 372, 618-622	33.3	101
141	Redox-couple investigations in Si-doped Li-rich cathode materials. *Physical Chemistry Chemical Physics*, **2021**, 23, 2780-2791	3.6	3
140	Dendrite-free Lithium Based on Lessons Learned from Lithium and Magnesium Electrodeposition Morphology Simulations. *Cell Reports Physical Science*, **2021**, 2, 100294	6.1	6
139	Modeling the electrical double layer at solid-state electrochemical interfaces. *Nature Computational Science*, **2021**, 1, 212-220		11
138	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	3.8	7
137	Reversible planar gliding and microcracking in a single-crystalline Ni-rich cathode. *Science*, **2020**, 370, 1313-1317	33.3	185
136	Evaluation of The Electrochemo-Mechanically Induced Stress in All-Solid-State Li-Ion Batteries. *Journal of the Electrochemical Society*, **2020**, 167, 090541	3.9	20
135	Efficient Low-Temperature Cycling of Lithium Metal Anodes by Tailoring the Solid-Electrolyte Interphase. *ACS Energy Letters*, **2020**, 5, 2411-2420	20.1	69
134	Compositions and Formation Mechanisms of Solid-Electrolyte Interphase on Microporous Carbon/Sulfur Cathodes. *Chemistry of Materials*, **2020**, 32, 3765-3775	9.6	17
133	Composition, crystallography, and oxygen vacancy ordering impacts on the oxygen ion conductivity of lanthanum strontium ferrite. *Physical Chemistry Chemical Physics*, **2020**, 22, 9723-9733	3.6	5
132	The origin of the two-plateaued or one-plateaued open circuit voltage in Li-S batteries. *Nano Energy*, **2020**, 75, 104915	17.1	10
131	Enhanced liquid metal wetting on oxide surfaces via patterned particles. *Acta Materialia*, **2020**, 199, 551-560	8.4	7
130	Optimization of the Reax force field for the lithium-oxygen system using a high fidelity charge model. *Journal of Chemical Physics*, **2020**, 153, 084107	3.9	5

129	A New General Paradigm for Understanding and Preventing Li Metal Penetration through Solid Electrolytes. *Joule*, **2020**, 4, 2599-2608	27.8	28
128	Wavelet scattering networks for atomistic systems with extrapolation of material properties. *Journal of Chemical Physics*, **2020**, 153, 084109	3.9	4
127	The Bonding Nature and Adhesion of Polyacrylic Acid Coating on Li-Metal for Li Dendrite Prevention. *ACS Applied Materials & Interfaces*, **2020**, 12, 51007-51015	9.5	8
126	How Transition Metals Enable Electron Transfer through the SEI: Part I. Experiments and Butler-Volmer Modeling. *Journal of the Electrochemical Society*, **2020**, 167, 013502	3.9	13
125	Mechanical and Electronic Stabilization of Solid Electrolyte Interphase with Sulfite Additive for Lithium Metal Batteries. *Journal of the Electrochemical Society*, **2019**, 166, A3201-A3206	3.9	4
124	First-Principles Prediction of Potentials and Space-Charge Layers in All-Solid-State Batteries. *Physical Review Letters*, **2019**, 122, 167701	7.4	38
123	Energy landscape of the charge transfer reaction at the complex Li/SEI/electrolyte interface. *Energy and Environmental Science*, **2019**, 12, 1286-1295	35.4	53
122	Connecting Oxide Bifilms□Properties from Atomistic Simulations with Virtual Casting of Aluminum. *Minerals, Metals and Materials Series*, **2019**, 45-51	0.3	1
121	Interfacial Electronic Properties Dictate Li Dendrite Growth in Solid Electrolytes. *Chemistry of Materials*, **2019**, 31, 7351-7359	9.6	80
120	Cathode porosity is a missing key parameter to optimize lithium-sulfur battery energy density. *Nature Communications*, **2019**, 10, 4597	17.4	91
119	High-Energy Rechargeable Metallic Lithium Battery at □70 □C Enabled by a Cosolvent Electrolyte. *Angewandte Chemie*, **2019**, 131, 5679-5683	3.6	38
118	High-Energy Rechargeable Metallic Lithium Battery at -70 □C Enabled by a Cosolvent Electrolyte. *Angewandte Chemie - International Edition*, **2019**, 58, 5623-5627	16.4	97
117	Adsorption of Lignin □O-4 Dimers on Metal Surfaces in Vacuum and Solvated Environments. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 2667-2678	8.3	7
116	Atomistic simulation of the formation and fracture of oxide bifilms in cast aluminum. *Acta Materialia*, **2019**, 164, 673-682	8.4	17
115	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	8.4	27
114	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	11.5	40
113	Nanoscale Protection Layers To Mitigate Degradation in High-Energy Electrochemical Energy Storage Systems. *Accounts of Chemical Research*, **2018**, 51, 97-106	24.3	25
112	Transferable Self-Consistent Charge Density Functional Tight-Binding Parameters for Li□Metal and Li-Ions in Inorganic Compounds and Organic Solvents. *Journal of Physical Chemistry C*, **2018**, 122, 10755-10764	3.8	12

111	Review on modeling of the anode solid electrolyte interphase (SEI) for lithium-ion batteries. *Npj Computational Materials*, **2018**, 4,	10.9	589
110	Si-doped high-energy Li1.2Mn0.54Ni0.13Co0.13O2 cathode with improved capacity for lithium-ion batteries. *Journal of Materials Research*, **2018**, 33, 4182-4191	2.5	6
109	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	6.4	19
108	Anisotropic chemical strain in cubic ceria due to oxygen-vacancy-induced elastic dipoles. *Physical Chemistry Chemical Physics*, **2018**, 20, 15293-15299	3.6	16
107	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	8.9	94
106	Atomistic Origin of Deformation Twinning in Biomineral Aragonite. *Physical Review Letters*, **2017**, 118, 105501	7.4	22
105	Atomistic Simulation Derived Insight on the Irreversible Structural Changes of Si Electrode during Fast and Slow Delithiation. *Nano Letters*, **2017**, 17, 4330-4338	11.5	29
104	Long-range charge transfer and oxygen vacancy interactions in strontium ferrite. *Journal of Materials Chemistry A*, **2017**, 5, 4493-4506	13	45
103	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	3.8	4
102	In situ stress measurements during electrochemical cycling of lithium-rich cathodes. *Journal of Power Sources*, **2017**, 364, 383-391	8.9	15
101	Computationally Driven Two-Dimensional Materials Design: What Is Next?. *ACS Nano*, **2017**, 11, 7560-7564	16.7	32
100	First-Principles Studies of Oxygen Vacancy Interactions and Their Impact on Oxygen Migration in Lanthanum Strontium Ferrite. *ECS Transactions*, **2017**, 78, 2807-2814	1	5
99	Polaron size and shape effects on oxygen vacancy interactions in lanthanum strontium ferrite. *Journal of Materials Chemistry A*, **2017**, 5, 25031-25043	13	20
98	How Solid-Electrolyte Interphase Forms in Aqueous Electrolytes. *Journal of the American Chemical Society*, **2017**, 139, 18670-18680	16.4	227
97	Simulation of the Effect of Contact Area Loss in All-Solid-State Li-Ion Batteries. *Journal of the Electrochemical Society*, **2017**, 164, E3512-E3521	3.9	75
96	Ab initio diffuse-interface model for lithiated electrode interface evolution. *Physical Review E*, **2016**, 94, 012802	2.4	5
95	Stabilizing high voltage LiCoO2 cathode in aqueous electrolyte with interphase-forming additive. *Energy and Environmental Science*, **2016**, 9, 3666-3673	35.4	140
94	Computational Analysis of Coupled Anisotropic Chemical Expansion in Li2-XMnO3-□ *MRS Advances*, **2016**, 1, 1037-1042	0.7	3

93	Self-generated concentration and modulus gradient coating design to protect Si nano-wire electrodes during lithiation. *Physical Chemistry Chemical Physics*, **2016**, 18, 3706-15	3.6	34
92	Interfacial Study on Solid Electrolyte Interphase at Li Metal Anode: Implication for Li Dendrite Growth. *Journal of the Electrochemical Society*, **2016**, 163, A592-A598	3.9	125
91	The impact of oxygen vacancies on lithium vacancy formation and diffusion in Li2-MnO3-. *Solid State Ionics*, **2016**, 289, 87-94	3.3	13
90	Design of Nanostructured Heterogeneous Solid Ionic Coatings through a Multiscale Defect Model. *ACS Applied Materials & Interfaces*, **2016**, 8, 5687-93	9.5	42
89	Synergetic Effects of Inorganic Components in Solid Electrolyte Interphase on High Cycle Efficiency of Lithium Ion Batteries. *Nano Letters*, **2016**, 16, 2011-6	11.5	219
88	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	8.9	132
87	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, 2114-27	2.8	64
86	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	24.3	93
85	Dissecting graphene capacitance in electrochemical cell. *Electrochimica Acta*, **2015**, 163, 296-302	6.7	16
84	General method to predict voltage-dependent ionic conduction in a solid electrolyte coating on electrodes. *Physical Review B*, **2015**, 91,	3.3	94
83	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	3.8	13
82	Diffusion-Induced Stress within Core-Shell Structures and Implications for Robust Electrode Design and Materials Selection. *Advances in Electrochemical Science and Engineering*, **2015**, 193-226		5
81	Modulation of dendritic patterns during electrodeposition: A nonlinear phase-field model. *Journal of Power Sources*, **2015**, 300, 376-385	8.9	125
80	Unveiling the environment-dependent mechanical properties of porous polypropylene separators. *Polymer*, **2014**, 55, 6282-6292	3.9	41
79	Introduction to Mechano-Electro-Chemical Coupling in Energy Related Materials and Devices. *Journal of the Electrochemical Society*, **2014**, 161, Y11-Y12	3.9	9
78	Deformation and fracture behaviors of microporous polymer separators for lithium ion batteries. *RSC Advances*, **2014**, 4, 14904	3.7	50
77	Property Evolution of Al2O3 Coated and Uncoated Si Electrodes: A First Principles Investigation. *Journal of the Electrochemical Society*, **2014**, 161, F3137-F3143	3.9	34
76	From ab initio calculations to multiscale design of Si/C core-shell particles for Li-ion anodes. *Nano Letters*, **2014**, 14, 2140-9	11.5	27

75	Oxidation-assisted ductility of aluminium nanowires. *Nature Communications*, **2014**, 5, 3959	17.4	55
74	Probing the Roles of Polymeric Separators in Lithium-Ion Battery Capacity Fade at Elevated Temperatures. *Journal of the Electrochemical Society*, **2014**, 161, A1241-A1246	3.9	22
73	Lithium Concentration Dependent Elastic Properties of Battery Electrode Materials from First Principles Calculations. *Journal of the Electrochemical Society*, **2014**, 161, F3010-F3018	3.9	167
72	Understanding and Predicting the Lithium Dendrite Formation in Li-Ion Batteries: Phase Field Model. *ECS Transactions*, **2014**, 61, 1-9	1	5
71	On the La2/3Li3xTiO3/Al2O3 composite solid-electrolyte for Li-ion conduction. *Journal of Alloys and Compounds*, **2013**, 577, 57-63	5.7	28
70	Improving microstructure of silicon/carbon nanofiber composites as a Li battery anode. *Journal of Power Sources*, **2013**, 221, 455-461	8.9	50
69	Oxidation induced softening in Al nanowires. *Applied Physics Letters*, **2013**, 102, 051912	3.4	36
68	Unveiling the Roles of Binder in the Mechanical Integrity of Electrodes for Lithium-Ion Batteries. *Journal of the Electrochemical Society*, **2013**, 160, A1502-A1509	3.9	107
67	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	4.4	34
66	A beaded-string silicon anode. *ACS Nano*, **2013**, 7, 2717-24	16.7	65
65	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	3.8	177
64	Li segregation induces structure and strength changes at the amorphous Si/Cu interface. *Nano Letters*, **2013**, 13, 4759-68	11.5	68
63	Conductivity of an atomically defined metallic interface. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 19097-102	11.5	24
62	Chemically Induced Crack Instability When Electrodes Fracture. *Journal of the Electrochemical Society*, **2012**, 159, A1838-A1843	3.9	20
61	Visualizing the chemistry and structure dynamics in lithium-ion batteries by in-situ neutron diffraction. *Scientific Reports*, **2012**, 2, 747	4.9	118
60	Lattice dynamics, thermodynamics and elastic properties of monoclinic Li2CO3 from density functional theory. *Acta Materialia*, **2012**, 60, 5204-5216	8.4	58
59	Direct calculation of Li-ion transport in the solid electrolyte interphase. *Journal of the American Chemical Society*, **2012**, 134, 15476-87	16.4	381
58	Stress Contributions to Solution Thermodynamics in Li-Si Alloys. *Electrochemical and Solid-State Letters*, **2012**, 15, A9		63

57	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		4
56	Nonlinear phase-field model for electrode-electrolyte interface evolution. *Physical Review E*, **2012**, 86, 051609	2.4	70
55	The mixing mechanism during lithiation of Si negative electrode in Li-ion batteries: an ab initio molecular dynamics study. *Nano Letters*, **2011**, 11, 5494-500	11.5	137
54	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, 14741-54	16.4	152
53	Role of oxygen and humidity on the tribo-chemical behaviour of non-hydrogenated diamond-like carbon coatings. *Wear*, **2011**, 271, 2157-2163	3.5	50
52	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	2.3	23
51	Material transfer mechanisms between aluminum and fluorinated carbon interfaces. *Acta Materialia*, **2011**, 59, 2601-2614	8.4	45
50	Mesoscale modeling of the influence of morphology on the mechanical properties of proton exchange membranes. *Polymer*, **2011**, 52, 201-210	3.9	20
49	First-principles study of void induced stresses at a diamond (100) grain boundary. *Journal of Applied Physics*, **2011**, 109, 033518	2.5	4
48	Environmental conditions to achieve low adhesion and low friction on diamond surfaces. *Modelling and Simulation in Materials Science and Engineering*, **2010**, 18, 034008	2	33
47	Mesopores inside electrode particles can change the Li-ion transport mechanism and diffusion-induced stress. *Journal of Materials Research*, **2010**, 25, 1433-1440	2.5	68
46	Adhesion at diamond/metal interfaces: A density functional theory study. *Journal of Applied Physics* , **2010**, 107, 033722	2.5	33
45	Effects of Concentration-Dependent Elastic Modulus on Diffusion-Induced Stresses for Battery Applications. *Journal of the Electrochemical Society*, **2010**, 157, A967	3.9	130
44	Threefold Increase in the Young□ Modulus of Graphite Negative Electrode during Lithium Intercalation. *Journal of the Electrochemical Society*, **2010**, 157, A558	3.9	281
43	In Situ Observation of Strains during Lithiation of a Graphite Electrode. *Journal of the Electrochemical Society*, **2010**, 157, A741	3.9	170
42	Elastic softening of amorphous and crystalline Li□i Phases with increasing Li concentration: A first-principles study. *Journal of Power Sources*, **2010**, 195, 6825-6830	8.9	316
41	Aluminum □ grain boundary sliding enhanced by vacancy diffusion. *Acta Materialia*, **2010**, 58, 4245-4252	8.4	18
40	Enhance diamond coating adhesion by oriented interlayer microcracking. *Journal of Applied Physics*, **2009**, 106, 123514	2.5	1

39	Surface stability and electronic structure of hydrogen- and fluorine-terminated diamond surfaces: A first principles investigation. *Journal of Materials Research*, **2009**, 24, 2461-2470	2.5	34
38	Engineering size-scaling of plastic deformation in nanoscale asperities. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 9580-5	11.5	21
37	Phase transition and morphology of polydispersed ABA(') triblock copolymers determined by continuous and discrete simulations. *Journal of Chemical Physics*, **2009**, 130, 064902	3.9	10
36	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	5.3	9
35	Strength characterization of Al/Si interfaces: A hybrid method of nanoindentation and finite element analysis. *Acta Materialia*, **2009**, 57, 695-707	8.4	24
34	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, 033101	2.5	45
33	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, 10195-203	3.6	12
32	Surface Stability and Electronic Structure of Hydrogen and Fluorine Terminated Diamond Surfaces: A First Principles Investigation. *Materials Research Society Symposia Proceedings*, **2008**, 1130, 63001		
31	Predicting the hydrogen pressure to achieve ultralow friction at diamond and diamondlike carbon surfaces from first principles. *Applied Physics Letters*, **2008**, 92, 241921	3.4	27
30	Intrinsic stress evolution in nanocrystalline diamond thin films with deposition temperature. *Applied Physics Letters*, **2008**, 92, 131908	3.4	25
29	Critical shear stresses at aluminum□silicon interfaces. *Acta Materialia*, **2008**, 56, 3461-3469	8.4	28
28	Ab initio study of the effect of solute atoms on the stacking fault energy in aluminum. *Physical Review B*, **2007**, 75,	3.3	75
27	Molecular dynamics simulations of grain boundary sliding: The effect of stress and boundary misorientation. *Acta Materialia*, **2007**, 55, 1555-1563	8.4	80
26	Origin of static friction and its relationship to adhesion at the atomic scale. *Physical Review B*, **2007**, 75,	3.3	26
25	Elucidating the contact mechanics of aluminum silicon surfaces with Green's function molecular dynamics. *Journal of Applied Physics*, **2007**, 102, 113511	2.5	8
24	Planar stacking effect on elastic stability of hexagonal boron nitride. *Applied Physics Letters*, **2007**, 90, 081922	3.4	35
23	Partial-mediated slips in nanocrystalline Ni at high strain rate. *Applied Physics Letters*, **2007**, 90, 221911	3.4	33
22	Mesoscale simulation of morphology in hydrated perfluorosulfonic acid membranes. *Journal of Chemical Physics*, **2006**, 124, 134702	3.9	157

21	Mechanical behavior of aluminum–silicon nanocomposites: A molecular dynamics study. *Acta Materialia*, **2006**, 54, 4441-4451	8.4	47
20	Aluminum–silicon interfaces and nanocomposites: A molecular dynamics study. *Composites Science and Technology*, **2006**, 66, 1151-1161	8.6	33
19	Atmospheric effects on the adhesion and friction between non-hydrogenated diamond-like carbon (DLC) coating and aluminum □A first principles investigation. *Surface Science*, **2006**, 600, 2955-2965	1.8	136
18	Atomic simulations of kinetic friction and its velocity dependence at Al□Al and □Al2O3□Al2O3 interfaces. *Physical Review B*, **2005**, 72,	3.3	37
17	A first principles study of adhesion and adhesive transfer at Al(111)/graphite(0001). *Surface Science* , **2005**, 581, 155-168	1.8	39
16	Adhesion and nonwetting-wetting transition in the Al/□Al2O3 interface. *Physical Review B*, **2004**, 69,	3.3	158
15	Adhesion and adhesive transfer at aluminum/diamond interfaces: A first-principles study. *Physical Review B*, **2004**, 69,	3.3	105
14	Hydrogen effect on adhesion and adhesive transfer at aluminum/diamond interfaces. *Physical Review B*, **2003**, 68,	3.3	44
13	Friction anisotropy at Ni(100)/(100) interfaces: Molecular dynamics studies. *Physical Review B*, **2002**, 66,	3.3	49
12	First principles multiscale modeling of physico-chemical aspects of tribology. *Tribology Series*, **2001**, 15-33		
11	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	5.3	21
10	MPiSIM: Massively parallel simulation tool for metallic system. *Journal of Computer-Aided Materials Design*, **2001**, 8, 185-192		2
9	Viscosities of liquid metal alloys from nonequilibrium molecular dynamics. *Journal of Computer-Aided Materials Design*, **2001**, 8, 233-243		71
8	Melting and crystallization in Ni nanoclusters: The mesoscale regime. *Journal of Chemical Physics*, **2001**, 115, 385-394	3.9	314
7	Molecular Dynamics Simulations of Supercooled Liquid Metals and Glasses. *Materials Research Society Symposia Proceedings*, **2000**, 644, 231		2
6	Molecular-dynamics simulations of glass formation and crystallization in binary liquid metals: Cu-Ag and Cu-Ni. *Physical Review B*, **1999**, 59, 3527-3533	3.3	228
5	Computational Materials Chemistry at the Nanoscale. *Journal of Nanoparticle Research*, **1999**, 1, 51-69	2.3	19
4	Strain Rate Induced Amorphization in Metallic Nanowires. *Physical Review Letters*, **1999**, 82, 2900-2903	7.4	246

3	Calculation of Mechanical, Thermodynamic and Transport Properties of Metallic Glass Formers. *Materials Research Society Symposia Proceedings*, **1998**, 554, 43		101
2	Deformation Behavior of FCC Crystalline Metallic Nanowires Under High Strain Rates. *Materials Research Society Symposia Proceedings*, **1998**, 554, 367		1
1	Spatially Resolved Potential and Li-Ion Distributions Reveal Performance-Limiting Regions in Solid-State Batteries. *ACS Energy Letters*,3944-3951	20.1	4