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	Review on modeling of the anode solid electrolyte interphase (SEI) for lithium-ion batteries. Npj Computational Materials, 2018, 4, .	8.7	961
2	Direct Calculation of Li-Ion Transport in the Solid Electrolyte Interphase. Journal of the American Chemical Society, 2012, 134, 15476-15487.	13.7	524
3	Reversible planar gliding and microcracking in a single-crystalline Ni-rich cathode. Science, 2020, 370, 1313-1317.	12.6	472
4	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
5	How Solid-Electrolyte Interphase Forms in Aqueous Electrolytes. Journal of the American Chemical Society, 2017, 139, 18670-18680.	13.7	365
6	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
7	Melting and crystallization in Ni nanoclusters: The mesoscale regime. Journal of Chemical Physics, 2001, 115, 385-394.	3.0	345
8	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
9	Interfacial toughening with self-assembled monolayers enhances perovskite solar cell reliability. Science, 2021, 372, 618-622.	12.6	313
10	Strain Rate Induced Amorphization in Metallic Nanowires. Physical Review Letters, 1999, 82, 2900-2903.	7.8	268
11	Copper-coordinated cellulose ion conductors for solid-state batteries. Nature, 2021, 598, 590-596.	27.8	262
12	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
13	Modulation of dendritic patterns during electrodeposition: A nonlinear phase-field model. Journal of Power Sources, 2015, 300, 376-385.	7.8	235
14	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
15	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
16	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
17	In Situ Observation of Strains during Lithiation of a Graphite Electrode. Journal of the Electrochemical Society, 2010, 157, A741.	2.9	205
18	Stabilizing high voltage LiCoO₂ cathode in aqueous electrolyte with interphase-forming additive. Energy and Environmental Science, 2016, 9, 3666-3673.	30.8	190

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19	Adhesion and nonwetting-wetting transition in theAl/Î±â^'Al2O3interface. Physical Review B, 2004, 69, .	3.2	184
20	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
21	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
22	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
23	Efficient Low-Temperature Cycling of Lithium Metal Anodes by Tailoring the Solid-Electrolyte Interphase. ACS Energy Letters, 2020, 5, 2411-2420.	17.4	174
24	Mesoscale simulation of morphology in hydrated perfluorosulfonic acid membranes. Journal of Chemical Physics, 2006, 124, 134702.	3.0	168
25	Cathode porosity is a missing key parameter to optimize lithium-sulfur battery energy density. Nature Communications, 2019, 10, 4597.	12.8	166
26	Interfacial Electronic Properties Dictate Li Dendrite Growth in Solid Electrolytes. Chemistry of Materials, 2019, 31, 7351-7359.	6.7	165
27	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
28	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
29	Effects of Concentration-Dependent Elastic Modulus on Diffusion-Induced Stresses for Battery Applications. Journal of the Electrochemical Society, 2010, 157, A967.	2.9	145
30	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
31	General method to predict voltage-dependent ionic conduction in a solid electrolyte coating on electrodes. Physical Review B, 2015, 91, .	3.2	141
32	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
33	Visualizing the chemistry and structure dynamics in lithium-ion batteries by in-situ neutron diffraction. Scientific Reports, 2012, 2, 747.	3.3	134
34	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
35	Adhesion and adhesive transfer at aluminum/diamond interfaces:â€,A first-principles study. Physical Review B, 2004, 69, .	3.2	118
36	Calculation of Mechanical, Thermodynamic and Transport Properties of Metallic Glass Formers. Materials Research Society Symposia Proceedings, 1998, 554, 43.	0.1	117

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37	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
38	Nonlinear phase-field model for electrode-electrolyte interface evolution. Physical Review E, 2012, 86, 051609.	2.1	100
39	Ab initiostudy of the effect of solute atoms on the stacking fault energy in aluminum. Physical Review B, 2007, 75, .	3.2	94
40	Molecular dynamics simulations of grain boundary sliding: The effect of stress and boundary misorientation. Acta Materialia, 2007, 55, 1555-1563.	7.9	93
41	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
42	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
43	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
44	Viscosities of liquid metal alloys from nonequilibrium molecular dynamics. Journal of Computer-Aided Materials Design, 2001, 8, 233-243.	0.7	79
45	Li Segregation Induces Structure and Strength Changes at the Amorphous Si/Cu Interface. Nano Letters, 2013, 13, 4759-4768.	9.1	75
46	A New General Paradigm for Understanding and Preventing Li Metal Penetration through Solid Electrolytes. Joule, 2020, 4, 2599-2608.	24.0	71
47	Stress Contributions to Solution Thermodynamics in Li-Si Alloys. Electrochemical and Solid-State Letters, 2012, 15, A9.	2.2	70
48	Long-range charge transfer and oxygen vacancy interactions in strontium ferrite. Journal of Materials Chemistry A, 2017, 5, 4493-4506.	10.3	69
49	A Beaded-String Silicon Anode. ACS Nano, 2013, 7, 2717-2724.	14.6	68
50	Oxidation-assisted ductility of aluminium nanowires. Nature Communications, 2014, 5, 3959.	12.8	66
51	Lattice dynamics, thermodynamics and elastic properties of monoclinic Li2CO3 from density functional theory. Acta Materialia, 2012, 60, 5204-5216.	7.9	64
52	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
53	Deformation and fracture behaviors of microporous polymer separators for lithium ion batteries. RSC Advances, 2014, 4, 14904.	3.6	57
54	First-Principles Prediction of Potentials and Space-Charge Layers in All-Solid-State Batteries. Physical Review Letters, 2019, 122, 167701.	7.8	57

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55	Friction anisotropy at Ni(100)/(100) interfaces:â€ƒMolecular dynamics studies. Physical Review B, 2002, 66, .	3.2	55
56	Mechanical behavior of aluminumâ€“silicon nanocomposites: A molecular dynamics study. Acta Materialia, 2006, 54, 4441-4451.	7.9	54
57	Unveiling the environment-dependent mechanical properties of porous polypropylene separators. Polymer, 2014, 55, 6282-6292.	3.8	54
58	Design of Nanostructured Heterogeneous Solid Ionic Coatings through a Multiscale Defect Model. ACS Applied Materials & Interfaces, 2016, 8, 5687-5693.	8.0	53
59	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
60	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
61	Improving microstructure of silicon/carbon nanofiber composites as a Li battery anode. Journal of Power Sources, 2013, 221, 455-461.	7.8	50
62	A high-performance hydroxide exchange membrane enabled by Cu2+-crosslinked chitosan. Nature Nanotechnology, 2022, 17, 629-636.	31.5	50
63	Material transfer mechanisms between aluminum and fluorinated carbon interfaces. Acta Materialia, 2011, 59, 2601-2614.	7.9	49
64	A first principles study of adhesion and adhesive transfer at Al(111)/graphite(0001). Surface Science, 2005, 581, 155-168.	1.9	47
65	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
66	Hydrogen effect on adhesion and adhesive transfer at aluminum/diamond interfaces. Physical Review B, 2003, 68, .	3.2	46
67	Adhesion at diamond/metal interfaces: A density functional theory study. Journal of Applied Physics, 2010, 107, .	2.5	46
68	Aluminumâ€“silicon interfaces and nanocomposites: A molecular dynamics study. Composites Science and Technology, 2006, 66, 1151-1161.	7.8	44
69	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
70	Atomic simulations of kinetic friction and its velocity dependence atAlâˆ•AlandÎ±â˜’Al2O3âˆ•Î±â˜’Al2O3interfaces. Physical Review B, 2005, 72, .	3.2	42
71	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
72	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

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73	Computationally Driven Two-Dimensional Materials Design: What Is Next?. ACS Nano, 2017, 11, 7560-7564.	14.6	39
74	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
75	Planar stacking effect on elastic stability of hexagonal boron nitride. Applied Physics Letters, 2007, 90, 081922.	3.3	38
76	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
77	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
78	Partial-mediated slips in nanocrystalline Ni at high strain rate. Applied Physics Letters, 2007, 90, 221911.	3.3	36
79	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
80	Oxidation induced softening in Al nanowires. Applied Physics Letters, 2013, 102, .	3.3	36
81	Property Evolution of Al₂O₃Coated and Uncoated Si Electrodes: A First Principles Investigation. Journal of the Electrochemical Society, 2014, 161, F3137-F3143.	2.9	36
82	Critical shear stresses at aluminumâ€“silicon interfaces. Acta Materialia, 2008, 56, 3461-3469.	7.9	35
83	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
84	Atomistic simulation of the formation and fracture of oxide bifilms in cast aluminum. Acta Materialia, 2019, 164, 673-682.	7.9	35
85	Modeling the electrical double layer at solid-state electrochemical interfaces. Nature Computational Science, 2021, 1, 212-220.	8.0	35
86	Nanoscale Protection Layers To Mitigate Degradation in High-Energy Electrochemical Energy Storage Systems. Accounts of Chemical Research, 2018, 51, 97-106.	15.6	33
87	Strength characterization of Al/Si interfaces: A hybrid method of nanoindentation and finite element analysis. Acta Materialia, 2009, 57, 695-707.	7.9	31
88	Origin of static friction and its relationship to adhesion at the atomic scale. Physical Review B, 2007, 75, .	3.2	30
89	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
90	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

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91	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
92	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
93	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
94	Intrinsic stress evolution in nanocrystalline diamond thin films with deposition temperature. Applied Physics Letters, 2008, 92, .	3.3	28
95	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
96	The origin of the two-plateaued or one-plateaued open circuit voltage in Liâ€“S batteries. Nano Energy, 2020, 75, 104915.	16.0	28
97	Compositions and Formation Mechanisms of Solid-Electrolyte Interphase on Microporous Carbon/Sulfur Cathodes. Chemistry of Materials, 2020, 32, 3765-3775.	6.7	27
98	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
99	Atomistic Origin of Deformation Twinning in Biomineral Aragonite. Physical Review Letters, 2017, 118, 105501.	7.8	25
100	Maintaining a Flat Li Surface during the Li Stripping Process via Interface Design. Chemistry of Materials, 2021, 33, 2814-2823.	6.7	25
101	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
102	Anisotropic chemical strain in cubic ceria due to oxygen-vacancy-induced elastic dipoles. Physical Chemistry Chemical Physics, 2018, 20, 15293-15299.	2.8	24
103	Computational Materials Chemistry at the Nanoscale. Journal of Nanoparticle Research, 1999, 1, 51-69.	1.9	23
104	Mesoscale modeling of the influence of morphology on the mechanical properties of proton exchange membranes. Polymer, 2011, 52, 201-210.	3.8	22
105	Chemically Induced Crack Instability When Electrodes Fracture. Journal of the Electrochemical Society, 2012, 159, A1838-A1843.	2.9	22
106	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
107	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
108	Aluminum Î£3 grain boundary sliding enhanced by vacancy diffusion. Acta Materialia, 2010, 58, 4245-4252.	7.9	21

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109	The impact of oxygen vacancies on lithium vacancy formation and diffusion in Li2-MnO3-. Solid State Ionics, 2016, 289, 87-94.	2.7	21
110	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
111	Dendrite-free Lithium Based on Lessons Learned from Lithium and Magnesium Electrodeposition Morphology Simulations. Cell Reports Physical Science, 2021, 2, 100294.	5.6	19
112	Dissecting graphene capacitance in electrochemical cell. Electrochimica Acta, 2015, 163, 296-302.	5.2	18
113	In situ stress measurements during electrochemical cycling of lithium-rich cathodes. Journal of Power Sources, 2017, 364, 383-391.	7.8	18
114	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
115	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
116	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
117	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
118	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
119	Understanding and Predicting the Lithium Dendrite Formation in Li-Ion Batteries: Phase Field Model. ECS Transactions, 2014, 61, 1-9.	0.5	13
120	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
121	Carbon-Nanotube-Encapsulated-Sulfur Cathodes for Lithiumâ€“Sulfur Batteries: Integrated Computational Design and Experimental Validation. Nano Letters, 2022, 22, 441-447.	9.1	12
122	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
123	Enhanced liquid metal wetting on oxide surfaces via patterned particles. Acta Materialia, 2020, 199, 551-560.	7.9	11
124	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
125	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
126	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

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127	Introduction to Mechano-Electro-Chemical Coupling in Energy Related Materials and Devices. Journal of the Electrochemical Society, 2014, 161, Y11-Y12.	2.9	9
128	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
129	Predicting low-impedance interfaces for solid-state batteries. Current Opinion in Solid State and Materials Science, 2022, 26, 100990.	11.5	9
130	Elucidating the contact mechanics of aluminum silicon surfaces with Green's function molecular dynamics. Journal of Applied Physics, 2007, 102, 113511.	2.5	8
131	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
132	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
133	Wavelet scattering networks for atomistic systems with extrapolation of material properties. Journal of Chemical Physics, 2020, 153, 084109.	3.0	8
134	Ab initiodiffuse-interface model for lithiated electrode interface evolution. Physical Review E, 2016, 94, 012802.	2.1	7
135	First-principles study of void induced stresses at a diamond (100) grain boundary. Journal of Applied Physics, 2011, 109, 033518.	2.5	6
136	Redox-couple investigations in Si-doped Li-rich cathode materials. Physical Chemistry Chemical Physics, 2021, 23, 2780-2791.	2.8	6
137	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
138	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
139	Computational Analysis of Coupled Anisotropic Chemical Expansion in Li2-XMnO3-Î´. MRS Advances, 2016, 1, 1037-1042.	0.9	4
140	Patterned nickel interlayers for enhanced silver wetting, spreading and adhesion on ceramic substrates. Scripta Materialia, 2021, 196, 113767.	5.2	4
141	Connecting Oxide Bifilmsâ€™ Properties from Atomistic Simulations with Virtual Casting of Aluminum. Minerals, Metals and Materials Series, 2019, , 45-51.	0.4	3
142	Molecular Dynamics Simulations of Supercooled Liquid Metals and Glasses. Materials Research Society Symposia Proceedings, 2000, 644, 231.	0.1	2
143	MPiSIM: Massively parallel simulation tool for metallic system. Journal of Computer-Aided Materials Design, 2001, 8, 185-192.	0.7	2
144	Enhance diamond coating adhesion by oriented interlayer microcracking. Journal of Applied Physics, 2009, 106, 123514.	2.5	2

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145	Deformation Behavior of FCC Crystalline Metallic Nanowires Under High Strain Rates. Materials Research Society Symposia Proceedings, 1998, 554, 367.	0.1	1
146	First principles multiscale modeling of physico-chemical aspects of tribology. Tribology Series, 2001, , 15-33.	0.1	1
147	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
148	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