

List of Publications by Citations

Source: <https://exaly.com/author-pdf/158363/yue-qi-publications-by-citations.pdf>
Version: 2024-04-09

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Review on modeling of the anode solid electrolyte interphase (SEI) for lithium-ion batteries. <i>Npj Computational Materials</i> , 2018 , 4,	10.9	589
145	Direct calculation of Li-ion transport in the solid electrolyte interphase. <i>Journal of the American Chemical Society</i> , 2012 , 134, 15476-87	16.4	381
144	Elastic softening of amorphous and crystalline LiBi Phases with increasing Li concentration: A first-principles study. <i>Journal of Power Sources</i> , 2010 , 195, 6825-6830	8.9	316
143	Melting and crystallization in Ni nanoclusters: The mesoscale regime. <i>Journal of Chemical Physics</i> , 2001 , 115, 385-394	3.9	314
142	Threefold Increase in the Young's Modulus of Graphite Negative Electrode during Lithium Intercalation. <i>Journal of the Electrochemical Society</i> , 2010 , 157, A558	3.9	281
141	Strain Rate Induced Amorphization in Metallic Nanowires. <i>Physical Review Letters</i> , 1999 , 82, 2900-2903	7.4	246
140	Molecular-dynamics simulations of glass formation and crystallization in binary liquid metals: Cu-Ag and Cu-Ni. <i>Physical Review B</i> , 1999 , 59, 3527-3533	3.3	228
139	How Solid-Electrolyte Interphase Forms in Aqueous Electrolytes. <i>Journal of the American Chemical Society</i> , 2017 , 139, 18670-18680	16.4	227
138	Synergetic Effects of Inorganic Components in Solid Electrolyte Interphase on High Cycle Efficiency of Lithium Ion Batteries. <i>Nano Letters</i> , 2016 , 16, 2011-6	11.5	219
137	Reversible planar gliding and microcracking in a single-crystalline Ni-rich cathode. <i>Science</i> , 2020 , 370, 1313-1317	33.3	185
136	Defect Thermodynamics and Diffusion Mechanisms in Li ₂ CO ₃ and Implications for the Solid Electrolyte Interphase in Li-Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 8579-8593	3.8	177
135	In Situ Observation of Strains during Lithiation of a Graphite Electrode. <i>Journal of the Electrochemical Society</i> , 2010 , 157, A741	3.9	170
134	Lithium Concentration Dependent Elastic Properties of Battery Electrode Materials from First Principles Calculations. <i>Journal of the Electrochemical Society</i> , 2014 , 161, F3010-F3018	3.9	167
133	Adhesion and nonwetting-wetting transition in the Al/Al ₂ O ₃ interface. <i>Physical Review B</i> , 2004 , 69,	3.3	158
132	Mesoscale simulation of morphology in hydrated perfluorosulfonic acid membranes. <i>Journal of Chemical Physics</i> , 2006 , 124, 134702	3.9	157
131	Using atomic layer deposition to hinder solvent decomposition in lithium ion batteries: first-principles modeling and experimental studies. <i>Journal of the American Chemical Society</i> , 2011 , 133, 14741-54	16.4	152
130	Stabilizing high voltage LiCoO ₂ cathode in aqueous electrolyte with interphase-forming additive. <i>Energy and Environmental Science</i> , 2016 , 9, 3666-3673	35.4	140

129	The mixing mechanism during lithiation of Si negative electrode in Li-ion batteries: an ab initio molecular dynamics study. <i>Nano Letters</i> , 2011 , 11, 5494-500	11.5	137
128	Atmospheric effects on the adhesion and friction between non-hydrogenated diamond-like carbon (DLC) coating and aluminum: A first principles investigation. <i>Surface Science</i> , 2006 , 600, 2955-2965	1.8	136
127	Connecting the irreversible capacity loss in Li-ion batteries with the electronic insulating properties of solid electrolyte interphase (SEI) components. <i>Journal of Power Sources</i> , 2016 , 309, 221-230	8.9	132
126	Effects of Concentration-Dependent Elastic Modulus on Diffusion-Induced Stresses for Battery Applications. <i>Journal of the Electrochemical Society</i> , 2010 , 157, A967	3.9	130
125	Interfacial Study on Solid Electrolyte Interphase at Li Metal Anode: Implication for Li Dendrite Growth. <i>Journal of the Electrochemical Society</i> , 2016 , 163, A592-A598	3.9	125
124	Modulation of dendritic patterns during electrodeposition: A nonlinear phase-field model. <i>Journal of Power Sources</i> , 2015 , 300, 376-385	8.9	125
123	Visualizing the chemistry and structure dynamics in lithium-ion batteries by in-situ neutron diffraction. <i>Scientific Reports</i> , 2012 , 2, 747	4.9	118
122	Unveiling the Roles of Binder in the Mechanical Integrity of Electrodes for Lithium-Ion Batteries. <i>Journal of the Electrochemical Society</i> , 2013 , 160, A1502-A1509	3.9	107
121	Adhesion and adhesive transfer at aluminum/diamond interfaces: A first-principles study. <i>Physical Review B</i> , 2004 , 69,	3.3	105
120	Calculation of Mechanical, Thermodynamic and Transport Properties of Metallic Glass Formers. <i>Materials Research Society Symposia Proceedings</i> , 1998 , 554, 43		101
119	Interfacial toughening with self-assembled monolayers enhances perovskite solar cell reliability. <i>Science</i> , 2021 , 372, 618-622	33.3	101
118	High-Energy Rechargeable Metallic Lithium Battery at -70 °C Enabled by a Cosolvent Electrolyte. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 5623-5627	16.4	97
117	General method to predict voltage-dependent ionic conduction in a solid electrolyte coating on electrodes. <i>Physical Review B</i> , 2015 , 91,	3.3	94
116	Computational study of lithium nucleation tendency in Li ₇ La ₃ Zr ₂ O ₁₂ (LLZO) and rational design of interlayer materials to prevent lithium dendrites. <i>Journal of Power Sources</i> , 2018 , 392, 79-86	8.9	94
115	Computational Exploration of the Li-Electrode Electrolyte Interface in the Presence of a Nanometer Thick Solid-Electrolyte Interphase Layer. <i>Accounts of Chemical Research</i> , 2016 , 49, 2363-2370	24.3	93
114	Cathode porosity is a missing key parameter to optimize lithium-sulfur battery energy density. <i>Nature Communications</i> , 2019 , 10, 4597	17.4	91
113	Interfacial Electronic Properties Dictate Li Dendrite Growth in Solid Electrolytes. <i>Chemistry of Materials</i> , 2019 , 31, 7351-7359	9.6	80
112	Molecular dynamics simulations of grain boundary sliding: The effect of stress and boundary misorientation. <i>Acta Materialia</i> , 2007 , 55, 1555-1563	8.4	80

111	Simulation of the Effect of Contact Area Loss in All-Solid-State Li-Ion Batteries. <i>Journal of the Electrochemical Society</i> , 2017 , 164, E3512-E3521	3.9	75
110	Ab initio study of the effect of solute atoms on the stacking fault energy in aluminum. <i>Physical Review B</i> , 2007 , 75,	3.3	75
109	Viscosities of liquid metal alloys from nonequilibrium molecular dynamics. <i>Journal of Computer-Aided Materials Design</i> , 2001 , 8, 233-243		71
108	Nonlinear phase-field model for electrode-electrolyte interface evolution. <i>Physical Review E</i> , 2012 , 86, 051609	2.4	70
107	Efficient Low-Temperature Cycling of Lithium Metal Anodes by Tailoring the Solid-Electrolyte Interphase. <i>ACS Energy Letters</i> , 2020 , 5, 2411-2420	20.1	69
106	Li segregation induces structure and strength changes at the amorphous Si/Cu interface. <i>Nano Letters</i> , 2013 , 13, 4759-68	11.5	68
105	Mesopores inside electrode particles can change the Li-ion transport mechanism and diffusion-induced stress. <i>Journal of Materials Research</i> , 2010 , 25, 1433-1440	2.5	68
104	A beaded-string silicon anode. <i>ACS Nano</i> , 2013 , 7, 2717-24	16.7	65
103	Atomic Insight into the Lithium Storage and Diffusion Mechanism of SiO ₂ /Al ₂ O ₃ Electrodes of Lithium Ion Batteries: ReaxFF Reactive Force Field Modeling. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 2114-27	2.8	64
102	Stress Contributions to Solution Thermodynamics in Li-Si Alloys. <i>Electrochemical and Solid-State Letters</i> , 2012 , 15, A9		63
101	Lattice dynamics, thermodynamics and elastic properties of monoclinic Li ₂ CO ₃ from density functional theory. <i>Acta Materialia</i> , 2012 , 60, 5204-5216	8.4	58
100	Oxidation-assisted ductility of aluminium nanowires. <i>Nature Communications</i> , 2014 , 5, 3959	17.4	55
99	Energy landscape of the charge transfer reaction at the complex Li/SEI/electrolyte interface. <i>Energy and Environmental Science</i> , 2019 , 12, 1286-1295	35.4	53
98	Deformation and fracture behaviors of microporous polymer separators for lithium ion batteries. <i>RSC Advances</i> , 2014 , 4, 14904	3.7	50
97	Improving microstructure of silicon/carbon nanofiber composites as a Li battery anode. <i>Journal of Power Sources</i> , 2013 , 221, 455-461	8.9	50
96	Role of oxygen and humidity on the tribo-chemical behaviour of non-hydrogenated diamond-like carbon coatings. <i>Wear</i> , 2011 , 271, 2157-2163	3.5	50
95	Friction anisotropy at Ni(100)/(100) interfaces: Molecular dynamics studies. <i>Physical Review B</i> , 2002 , 66,	3.3	49
94	Copper-coordinated cellulose ion conductors for solid-state batteries. <i>Nature</i> , 2021 , 598, 590-596	50.4	49

93	Mechanical behavior of aluminum/silicon nanocomposites: A molecular dynamics study. <i>Acta Materialia</i> , 2006 , 54, 4441-4451	8.4	47
92	Long-range charge transfer and oxygen vacancy interactions in strontium ferrite. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 4493-4506	13	45
91	Material transfer mechanisms between aluminum and fluorinated carbon interfaces. <i>Acta Materialia</i> , 2011 , 59, 2601-2614	8.4	45
90	A molecular dynamics simulation study of hydrated sulfonated poly(ether ether ketone) for application to polymer electrolyte membrane fuel cells: Effect of water content. <i>Journal of Renewable and Sustainable Energy</i> , 2009 , 1, 033101	2.5	45
89	Hydrogen effect on adhesion and adhesive transfer at aluminum/diamond interfaces. <i>Physical Review B</i> , 2003 , 68,	3.3	44
88	Design of Nanostructured Heterogeneous Solid Ionic Coatings through a Multiscale Defect Model. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 5687-93	9.5	42
87	Unveiling the environment-dependent mechanical properties of porous polypropylene separators. <i>Polymer</i> , 2014 , 55, 6282-6292	3.9	41
86	From Microparticles to Nanowires and Back: Radical Transformations in Plated Li Metal Morphology Revealed via in Situ Scanning Electron Microscopy. <i>Nano Letters</i> , 2018 , 18, 1644-1650	11.5	40
85	A first principles study of adhesion and adhesive transfer at Al(111)/graphite(0001). <i>Surface Science</i> , 2005 , 581, 155-168	1.8	39
84	First-Principles Prediction of Potentials and Space-Charge Layers in All-Solid-State Batteries. <i>Physical Review Letters</i> , 2019 , 122, 167701	7.4	38
83	High-Energy Rechargeable Metallic Lithium Battery at -70 °C Enabled by a Cosolvent Electrolyte. <i>Angewandte Chemie</i> , 2019 , 131, 5679-5683	3.6	38
82	Atomic simulations of kinetic friction and its velocity dependence at Al/Al and Al ₂ O ₃ /Al ₂ O ₃ interfaces. <i>Physical Review B</i> , 2005 , 72,	3.3	37
81	Oxidation induced softening in Al nanowires. <i>Applied Physics Letters</i> , 2013 , 102, 051912	3.4	36
80	Planar stacking effect on elastic stability of hexagonal boron nitride. <i>Applied Physics Letters</i> , 2007 , 90, 081922	3.4	35
79	Self-generated concentration and modulus gradient coating design to protect Si nano-wire electrodes during lithiation. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 3706-15	3.6	34
78	Property Evolution of Al ₂ O ₃ Coated and Uncoated Si Electrodes: A First Principles Investigation. <i>Journal of the Electrochemical Society</i> , 2014 , 161, F3137-F3143	3.9	34
77	Low friction and environmentally stable diamond-like carbon (DLC) coatings incorporating silicon, oxygen and fluorine sliding against aluminum. <i>Surface and Coatings Technology</i> , 2013 , 215, 340-349	4.4	34
76	Surface stability and electronic structure of hydrogen- and fluorine-terminated diamond surfaces: A first principles investigation. <i>Journal of Materials Research</i> , 2009 , 24, 2461-2470	2.5	34

75	Environmental conditions to achieve low adhesion and low friction on diamond surfaces. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010 , 18, 034008	2	33
74	Adhesion at diamond/metal interfaces: A density functional theory study. <i>Journal of Applied Physics</i> , 2010 , 107, 033722	2.5	33
73	Partial-mediated slips in nanocrystalline Ni at high strain rate. <i>Applied Physics Letters</i> , 2007 , 90, 221911	3.4	33
72	Aluminum/Silicon interfaces and nanocomposites: A molecular dynamics study. <i>Composites Science and Technology</i> , 2006 , 66, 1151-1161	8.6	33
71	Computationally Driven Two-Dimensional Materials Design: What Is Next?. <i>ACS Nano</i> , 2017 , 11, 7560-7566	6.7	32
70	Atomistic Simulation Derived Insight on the Irreversible Structural Changes of Si Electrode during Fast and Slow Delithiation. <i>Nano Letters</i> , 2017 , 17, 4330-4338	11.5	29
69	On the La ₂ /3xLi ₃ TiO ₃ /Al ₂ O ₃ composite solid-electrolyte for Li-ion conduction. <i>Journal of Alloys and Compounds</i> , 2013 , 577, 57-63	5.7	28
68	Critical shear stresses at aluminum/Silicon interfaces. <i>Acta Materialia</i> , 2008 , 56, 3461-3469	8.4	28
67	A New General Paradigm for Understanding and Preventing Li Metal Penetration through Solid Electrolytes. <i>Joule</i> , 2020 , 4, 2599-2608	27.8	28
66	Computational design of metal oxides to enhance the wetting and adhesion of silver-based brazes on yttria-stabilized-zirconia. <i>Acta Materialia</i> , 2018 , 152, 229-238	8.4	27
65	From ab initio calculations to multiscale design of Si/C core-shell particles for Li-ion anodes. <i>Nano Letters</i> , 2014 , 14, 2140-9	11.5	27
64	Predicting the hydrogen pressure to achieve ultralow friction at diamond and diamondlike carbon surfaces from first principles. <i>Applied Physics Letters</i> , 2008 , 92, 241921	3.4	27
63	Origin of static friction and its relationship to adhesion at the atomic scale. <i>Physical Review B</i> , 2007 , 75,	3.3	26
62	Nanoscale Protection Layers To Mitigate Degradation in High-Energy Electrochemical Energy Storage Systems. <i>Accounts of Chemical Research</i> , 2018 , 51, 97-106	24.3	25
61	Intrinsic stress evolution in nanocrystalline diamond thin films with deposition temperature. <i>Applied Physics Letters</i> , 2008 , 92, 131908	3.4	25
60	Conductivity of an atomically defined metallic interface. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 19097-102	11.5	24
59	Strength characterization of Al/Si interfaces: A hybrid method of nanoindentation and finite element analysis. <i>Acta Materialia</i> , 2009 , 57, 695-707	8.4	24
58	The Effect of Solute Atoms on Aluminum Grain Boundary Sliding at Elevated Temperature. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2011 , 42, 651-659	2.3	23

57	Atomistic Origin of Deformation Twinning in Biomineral Aragonite. <i>Physical Review Letters</i> , 2017 , 118, 105501	7.4	22
56	Probing the Roles of Polymeric Separators in Lithium-Ion Battery Capacity Fade at Elevated Temperatures. <i>Journal of the Electrochemical Society</i> , 2014 , 161, A1241-A1246	3.9	22
55	Engineering size-scaling of plastic deformation in nanoscale asperities. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009 , 106, 9580-5	11.5	21
54	Large scale atomistic simulations of screw dislocation structure, annihilation and cross-slip in FCC Ni. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2001 , 309-310, 156-159	5.3	21
53	Evaluation of The Electrochemo-Mechanically Induced Stress in All-Solid-State Li-Ion Batteries. <i>Journal of the Electrochemical Society</i> , 2020 , 167, 090541	3.9	20
52	Polaron size and shape effects on oxygen vacancy interactions in lanthanum strontium ferrite. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 25031-25043	13	20
51	Chemically Induced Crack Instability When Electrodes Fracture. <i>Journal of the Electrochemical Society</i> , 2012 , 159, A1838-A1843	3.9	20
50	Mesoscale modeling of the influence of morphology on the mechanical properties of proton exchange membranes. <i>Polymer</i> , 2011 , 52, 201-210	3.9	20
49	Computational Materials Chemistry at the Nanoscale. <i>Journal of Nanoparticle Research</i> , 1999 , 1, 51-69	2.3	19
48	A Bottom-Up Formation Mechanism of Solid Electrolyte Interphase Revealed by Isotope-Assisted Time-of-Flight Secondary Ion Mass Spectrometry. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 5508-5514	6.4	19
47	Aluminum β grain boundary sliding enhanced by vacancy diffusion. <i>Acta Materialia</i> , 2010 , 58, 4245-4252	8.4	18
46	Compositions and Formation Mechanisms of Solid-Electrolyte Interphase on Microporous Carbon/Sulfur Cathodes. <i>Chemistry of Materials</i> , 2020 , 32, 3765-3775	9.6	17
45	Atomistic simulation of the formation and fracture of oxide bifilms in cast aluminum. <i>Acta Materialia</i> , 2019 , 164, 673-682	8.4	17
44	Dissecting graphene capacitance in electrochemical cell. <i>Electrochimica Acta</i> , 2015 , 163, 296-302	6.7	16
43	Anisotropic chemical strain in cubic ceria due to oxygen-vacancy-induced elastic dipoles. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 15293-15299	3.6	16
42	In situ stress measurements during electrochemical cycling of lithium-rich cathodes. <i>Journal of Power Sources</i> , 2017 , 364, 383-391	8.9	15
41	Vacancies in Si Can Improve the Concentration-Dependent Lithiation Rate: Molecular Dynamics Studies of Lithiation Dynamics of Si Electrodes. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 24265-24275	3.8	13
40	The impact of oxygen vacancies on lithium vacancy formation and diffusion in Li ₂ -MnO ₃ -. <i>Solid State Ionics</i> , 2016 , 289, 87-94	3.3	13

- 39 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
- 38 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
- 37 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
- 36 Modeling the electrical double layer at solid-state electrochemical interfaces. *Nature Computational Science*, **2021**, 1, 212-220 11
- 35 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
- 34 The origin of the two-plateaued or one-plateaued open circuit voltage in LiB batteries. *Nano Energy*, **2020**, 75, 104915 17.1 10
- 33 Maintaining a Flat Li Surface during the Li Stripping Process via Interface Design. *Chemistry of Materials*, **2021**, 33, 2814-2823 9.6 10
- 32 Introduction to Mechano-Electro-Chemical Coupling in Energy Related Materials and Devices. *Journal of the Electrochemical Society*, **2014**, 161, Y11-Y12 3.9 9
- 31 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
- 30 Elucidating the contact mechanics of aluminum silicon surfaces with Green's function molecular dynamics. *Journal of Applied Physics*, **2007**, 102, 113511 2.5 8
- 29 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
- 28 Enhanced liquid metal wetting on oxide surfaces via patterned particles. *Acta Materialia*, **2020**, 199, 551-560 5.6 7
- 27 Adsorption of Lignin E-4 Dimers on Metal Surfaces in Vacuum and Solvated Environments. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 2667-2678 8.3 7
- 26 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
- 25 Dendrite-free Lithium Based on Lessons Learned from Lithium and Magnesium Electrodeposition Morphology Simulations. *Cell Reports Physical Science*, **2021**, 2, 100294 6.1 6
- 24 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 2.5 6
- 23 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
- 22 Ab initio diffuse-interface model for lithiated electrode interface evolution. *Physical Review E*, **2016**, 94, 012802 2.4 5

21	First-Principles Studies of Oxygen Vacancy Interactions and Their Impact on Oxygen Migration in Lanthanum Strontium Ferrite. <i>ECS Transactions</i> , 2017 , 78, 2807-2814	1	5
20	Diffusion-Induced Stress within Core/Shell Structures and Implications for Robust Electrode Design and Materials Selection. <i>Advances in Electrochemical Science and Engineering</i> , 2015 , 193-226		5
19	Understanding and Predicting the Lithium Dendrite Formation in Li-Ion Batteries: Phase Field Model. <i>ECS Transactions</i> , 2014 , 61, 1-9	1	5
18	Optimization of the Reax force field for the lithium-oxygen system using a high fidelity charge model. <i>Journal of Chemical Physics</i> , 2020 , 153, 084107	3.9	5
17	Mechanical and Electronic Stabilization of Solid Electrolyte Interphase with Sulfite Additive for Lithium Metal Batteries. <i>Journal of the Electrochemical Society</i> , 2019 , 166, A3201-A3206	3.9	4
16	Integrated Computation and Experimental Investigation on the Adsorption Mechanisms of Anti-Wear and Anti-Corrosion Additives on Copper. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 21995-22003	3.8	4
15	First-principles study of void induced stresses at a diamond (100) grain boundary. <i>Journal of Applied Physics</i> , 2011 , 109, 033518	2.5	4
14	Publisher's Note: Stress Contributions to Solution Thermodynamics in Li-Si Alloys [Electrochem. Solid-State Lett., 15, A9 (2012)]. <i>Electrochemical and Solid-State Letters</i> , 2012 , 15, S3		4
13	Spatially Resolved Potential and Li-Ion Distributions Reveal Performance-Limiting Regions in Solid-State Batteries. <i>ACS Energy Letters</i> , 2019 , 4, 3944-3951	20.1	4
12	Wavelet scattering networks for atomistic systems with extrapolation of material properties. <i>Journal of Chemical Physics</i> , 2020 , 153, 084109	3.9	4
11	Computational Analysis of Coupled Anisotropic Chemical Expansion in Li ₂ -XMnO ₃ . <i>MRS Advances</i> , 2016 , 1, 1037-1042	0.7	3
10	Redox-couple investigations in Si-doped Li-rich cathode materials. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 2780-2791	3.6	3
9	MPiSIM: Massively parallel simulation tool for metallic system. <i>Journal of Computer-Aided Materials Design</i> , 2001 , 8, 185-192		2
8	Molecular Dynamics Simulations of Supercooled Liquid Metals and Glasses. <i>Materials Research Society Symposia Proceedings</i> , 2000 , 644, 231		2
7	Connecting Oxide Bilayers Properties from Atomistic Simulations with Virtual Casting of Aluminum. <i>Minerals, Metals and Materials Series</i> , 2019 , 45-51	0.3	1
6	Enhance diamond coating adhesion by oriented interlayer microcracking. <i>Journal of Applied Physics</i> , 2009 , 106, 123514	2.5	1
5	Deformation Behavior of FCC Crystalline Metallic Nanowires Under High Strain Rates. <i>Materials Research Society Symposia Proceedings</i> , 1998 , 554, 367		1
4	Patterned nickel interlayers for enhanced silver wetting, spreading and adhesion on ceramic substrates. <i>Scripta Materialia</i> , 2021 , 196, 113767	5.6	1

- 3 Predicting low-impedance interfaces for solid-state batteries. *Current Opinion in Solid State and Materials Science*, **2022**, 26, 100990 12 1
- 2 Surface Stability and Electronic Structure of Hydrogen and Fluorine Terminated Diamond Surfaces: A First Principles Investigation. *Materials Research Society Symposia Proceedings*, **2008**, 1130, 63001
- 1 First principles multiscale modeling of physico-chemical aspects of tribology. *Tribology Series*, **2001**, 15-33