

# Katsuyo Thornton

## List of Publications by Year in descending order

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137  
papers

7,652  
citations

70961

41  
h-index

53109

85  
g-index

140  
all docs

140  
docs citations

140  
times ranked

9216  
citing authors

#	ARTICLE	IF	CITATIONS
1	Diffuse-charge dynamics in electrochemical systems. <i>Physical Review E</i> , 2004, 70, 021506.	0.8	822
2	Three-dimensional reconstruction of a solid-oxide fuel-cell anode. <i>Nature Materials</i> , 2006, 5, 541-544.	13.3	727
3	Dendrites and Pits: Untangling the Complex Behavior of Lithium Metal Anodes through Operando Video Microscopy. <i>ACS Central Science</i> , 2016, 2, 790-801.	5.3	662
4	Energy Input and Mass Redistribution by Supernovae in the Interstellar Medium. <i>Astrophysical Journal</i> , 1998, 500, 95-119.	1.6	352
5	New frontiers for the materials genome initiative. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	312
6	Tracking lithium transport and electrochemical reactions in nanoparticles. <i>Nature Communications</i> , 2012, 3, 1201.	5.8	254
7	Single-particle measurements of electrochemical kinetics in NMC and NCA cathodes for Li-ion batteries. <i>Energy and Environmental Science</i> , 2018, 11, 860-871.	15.6	224
8	Electrochemical Stability Window of Imidazolium-Based Ionic Liquids as Electrolytes for Lithium Batteries. <i>Journal of Physical Chemistry B</i> , 2016, 120, 5691-5702.	1.2	182
9	Efficient fast-charging of lithium-ion batteries enabled by laser-patterned three-dimensional graphite anode architectures. <i>Journal of Power Sources</i> , 2020, 471, 228475.	4.0	168
10	Quantitative three-dimensional microstructure of a solid oxide fuel cell cathode. <i>Electrochemistry Communications</i> , 2009, 11, 1052-1056.	2.3	141
11	Effect of composition of (La <sub>0.8</sub> Sr <sub>0.2</sub> MnO <sub>3</sub> â€“Y <sub>2</sub> O <sub>3</sub> -stabilized ZrO <sub>2</sub> ) cathodes: Correlating three-dimensional microstructure and polarization resistance. <i>Journal of Power Sources</i> , 2010, 195, 1829-1840.	4.0	139
12	Three-dimensional mesostructures as high-temperature growth templates, electronic cellular scaffolds, and self-propelled microrobots. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E9455-E9464.	3.3	129
13	Modelling the evolution of phase boundaries in solids at the meso- and nano-scales. <i>Acta Materialia</i> , 2003, 51, 5675-5710.	3.8	125
14	Enabling 6C Fast Charging of Li-ion Batteries with Graphite/Hard Carbon Hybrid Anodes. <i>Advanced Energy Materials</i> , 2021, 11, 2003336.	10.2	116
15	Simulation of coarsening in three-phase solid oxide fuel cell anodes. <i>Journal of Power Sources</i> , 2011, 196, 1333-1337.	4.0	105
16	Designing the next generation high capacity battery electrodes. <i>Energy and Environmental Science</i> , 2014, 7, 1760.	15.6	104
17	Vacancy mediated substitutional diffusion in binary crystalline solids. <i>Progress in Materials Science</i> , 2010, 55, 61-105.	16.0	95
18	Mapping the Inhomogeneous Electrochemical Reaction Through Porous LiFePO <sub>4</sub> -Electrodes in a Standard Coin Cell Battery. <i>Chemistry of Materials</i> , 2015, 27, 2374-2386.	3.2	93

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19	Tortuosity characterization of 3D microstructure at nano-scale for energy storage and conversion materials. <i>Journal of Power Sources</i> , 2014, 249, 349-356.	4.0	91
20	Extended smoothed boundary method for solving partial differential equations with general boundary conditions on complex boundaries. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2012, 20, 075008.	0.8	86
21	Quantum dot formation on a strain-patterned epitaxial thin film. <i>Applied Physics Letters</i> , 2005, 87, 133102.	1.5	75
22	Three-dimensional analysis of particle coarsening in high volume fraction solid-liquid mixtures. <i>Acta Materialia</i> , 2006, 54, 2027-2039.	3.8	74
23	X-ray micro-computed tomography and tortuosity calculations of percolating pore networks. <i>Acta Materialia</i> , 2014, 71, 126-135.	3.8	72
24	Particle-Level Modeling of the Charge-Discharge Behavior of Nanoparticulate Phase-Separating Li-Ion Battery Electrodes. <i>Journal of the Electrochemical Society</i> , 2014, 161, A535-A546.	1.3	69
25	Modeling fluid flow in three-dimensional single crystal dendritic structures. <i>Acta Materialia</i> , 2010, 58, 2864-2875.	3.8	64
26	Topological complexity and the dynamics of coarsening. <i>Nature Materials</i> , 2004, 3, 385-388.	13.3	61
27	The evolution of interfacial topology during coarsening. <i>Acta Materialia</i> , 2006, 54, 743-750.	3.8	58
28	Large-scale simulations of Ostwald ripening in elastically stressed solids: I. Development of microstructure. <i>Acta Materialia</i> , 2004, 52, 1353-1364.	3.8	57
29	Effects of Antisite Defects on Li Diffusion in $\text{LiFePO}_4$ Revealed by Li Isotope Exchange. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12025-12036.	1.5	55
30	<i>Operando</i> video microscopy of Li plating and re-intercalation on graphite anodes during fast charging. <i>Journal of Materials Chemistry A</i> , 2021, 9, 23522-23536.	5.2	54
31	Large-scale simulations of Ostwald ripening in elastically stressed solids. II. Coarsening kinetics and particle size distribution. <i>Acta Materialia</i> , 2004, 52, 1365-1378.	3.8	53
32	Computational materials science and engineering education: A survey of trends and needs. <i>Jom</i> , 2009, 61, 12-17.	0.9	51
33	Multifunctionality of three-dimensional self-assembled composite structure. <i>Scripta Materialia</i> , 2009, 61, 52-55.	2.6	50
34	Localized concentration reversal of lithium during intercalation into nanoparticles. <i>Science Advances</i> , 2018, 4, eaao2608.	4.7	50
35	Density-amplitude formulation of the phase-field crystal model for two-phase coexistence in two and three dimensions. <i>Philosophical Magazine</i> , 2010, 90, 237-263.	0.7	49
36	Particle-size and morphology dependence of the preferred interface orientation in $\text{LiFePO}_4$ nano-particles. <i>Journal of Materials Chemistry A</i> , 2014, 2, 15437-15447.	5.2	45

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37	Thermodynamic Overpotentials and Nucleation Rates for Electrodeposition on Metal Anodes. ACS Applied Materials & Interfaces, 2019, 11, 7954-7964.	4.0	44
38	Quantifying Reaction and Rate Heterogeneity in Battery Electrodes in 3D through Operando X-ray Diffraction Computed Tomography. ACS Applied Materials & Interfaces, 2019, 11, 18386-18394.	4.0	44
39	Coarsening of bicontinuous structures via nonconserved and conserved dynamics. Physical Review E, 2007, 75, 021120.	0.8	43
40	Architecture Dependence on the Dynamics of Nano-LiFePO <sub>4</sub> Electrodes. Electrochimica Acta, 2014, 137, 245-257.	2.6	43
41	Phase field modeling of solidification under stress. Physical Review B, 2006, 74, .	1.1	42
42	Morphology and topology in coarsening of domains via non-conserved and conserved dynamics. Philosophical Magazine, 2010, 90, 317-335.	0.7	42
43	The Kirkendall effect in the phase field crystal model. Philosophical Magazine, 2011, 91, 151-164.	0.7	41
44	High-Operating-Temperature Direct Ink Writing of Mesoscale Eutectic Architectures. Advanced Materials, 2017, 29, 1604778.	11.1	41
45	Theory of grain boundary diffusion induced by the Kirkendall effect. Applied Physics Letters, 2008, 93, .	1.5	38
46	Three-Dimensional Materials Science: An Intersection of Three-Dimensional Reconstructions and Simulations. MRS Bulletin, 2008, 33, 587-595.	1.7	38
47	Radiative effects in radiative shocks in shock tubes. High Energy Density Physics, 2011, 7, 130-140.	0.4	38
48	Large-Scale Simulations of Microstructural Evolution in Elastically Stressed Solids. Journal of Computational Physics, 2001, 173, 61-86.	1.9	37
49	Dynamics of Late-Stage Phase Separation in Crystalline Solids. Physical Review Letters, 2001, 86, 1259-1262.	2.9	37
50	Two- and three-dimensional equilibrium morphology of a misfitting particle and the Gibbs-Thomson effect. Acta Materialia, 2004, 52, 5829-5843.	3.8	37
51	Coupled composition-deformation phase-field method for multicomponent lipid membranes. Physical Review E, 2007, 76, 011912.	0.8	37
52	The topology and morphology of bicontinuous interfaces during coarsening. Europhysics Letters, 2009, 86, 46005.	0.7	37
53	Misfit-driven $\hat{\rho}^2$ precipitate composition and morphology in Mg-Nd alloys. Acta Materialia, 2017, 136, 378-389.	3.8	36
54	The dynamics of interfaces during coarsening in solid-liquid systems. Acta Materialia, 2014, 70, 66-78.	3.8	33

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55	PRISMS-PF: A general framework for phase-field modeling with a matrix-free finite element method. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	33
56	Rate Limitations in Composite Solid-State Battery Electrodes: Revealing Heterogeneity with <i>in situ</i> Operando Microscopy. <i>ACS Energy Letters</i> , 2021, 6, 2993-3003.	8.8	33
57	Numerical Modeling of Localized Corrosion Using Phase-Field and Smoothed Boundary Methods. <i>Journal of the Electrochemical Society</i> , 2018, 165, C633-C646.	1.3	32
58	Domain Growth in Ternary Fluids: A Level Set Approach. <i>Physical Review Letters</i> , 2000, 84, 91-94.	2.9	30
59	Fluid Flow and Defect Formation in the Three-Dimensional Dendritic Structure of Nickel-Based Single Crystals. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2012, 43, 369-380.	1.1	30
60	Calculations of isothermal elastic constants in the phase-field crystal model. <i>Physical Review B</i> , 2013, 87, .	1.1	30
61	General method for incorporating CALPHAD free energies of mixing into phase field models: Application to the $\text{Zr}$ -zirconium/ $\text{H}$ -hydride system. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2015, 51, 334-343.	0.7	30
62	PRISMS: An Integrated, Open-Source Framework for Accelerating Predictive Structural Materials Science. <i>Jom</i> , 2018, 70, 2298-2314.	0.9	30
63	Substitutional diffusion and Kirkendall effect in binary crystalline solids containing discrete vacancy sources and sinks. <i>Acta Materialia</i> , 2007, 55, 6690-6704.	3.8	29
64	Effect of a Size-Dependent Equilibrium Potential on Nano- $\text{LiFePO}_4$ Particle Interactions. <i>Journal of the Electrochemical Society</i> , 2015, 162, A1718-A1724.	1.3	29
65	The thermodynamic stability of intermediate solid solutions in $\text{LiFePO}_4$ nanoparticles. <i>Journal of Materials Chemistry A</i> , 2016, 4, 5436-5447.	5.2	29
66	Template-Directed Directionally Solidified 3D Mesostructured $\text{AgCl/KCl}$ Eutectic Photonic Crystals. <i>Advanced Materials</i> , 2015, 27, 4551-4559.	11.1	28
67	Kinetics of Nanoparticle Interactions in Battery Electrodes. <i>Journal of the Electrochemical Society</i> , 2015, 162, A965-A973.	1.3	28
68	A nucleation algorithm for the coupled conserved/nonconserved phase field model. <i>Computational Materials Science</i> , 2016, 112, 128-138.	1.4	26
69	Deformation and stresses in solid-state composite battery cathodes. <i>Journal of Power Sources</i> , 2019, 440, 227116.	4.0	26
70	Computational Model of Magnesium Deposition and Dissolution for Property Determination via Cyclic Voltammetry. <i>Journal of the Electrochemical Society</i> , 2016, 163, A1813-A1821.	1.3	21
71	Archimedean lattices emerge in template-directed eutectic solidification. <i>Nature</i> , 2020, 577, 355-358.	13.7	21
72	Computational Examination of Orientation-Dependent Morphological Evolution during the Electrodeposition and Electrodissolution of Magnesium. <i>Journal of the Electrochemical Society</i> , 2016, 163, A513-A521.	1.3	20

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73	Application of the level-set method to the analysis of an evolving microstructure. <i>Computational Materials Science</i> , 2014, 85, 46-58.	1.4	19
74	Morphological stability during electrodeposition. <i>MRS Communications</i> , 2017, 7, 658-663.	0.8	19
75	Template-Directed Solidification of Eutectic Optical Materials. <i>Advanced Optical Materials</i> , 2018, 6, 1800071.	3.6	19
76	A thermal-gradient approach to variable-temperature measurements resolved in space. <i>Journal of Applied Crystallography</i> , 2020, 53, 662-670.	1.9	19
77	Three Dimensional Reconstruction of Solid Oxide Fuel Cell Electrodes Using Focused Ion Beam - Scanning Electron Microscopy. <i>ECS Transactions</i> , 2007, 7, 1879-1887.	0.3	16
78	Modeling SOFC Cathodes Based on 3-D Representations of Electrode Microstructure. <i>ECS Transactions</i> , 2011, 35, 815-822.	0.3	16
79	Phase-field crystal model for a diamond-cubic structure. <i>Physical Review E</i> , 2015, 91, 053305.	0.8	16
80	Simulations of the Kirkendall-Effect-Induced Deformation of Thermodynamically Ideal Binary Diffusion Couples with General Geometries. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2012, 43, 3481-3500.	1.1	15
81	Coarsening of complex microstructures following spinodal decomposition. <i>Acta Materialia</i> , 2017, 132, 13-24.	3.8	15
82	Classical density functional theory and the phase-field crystal method using a rational function to describe the two-body direct correlation function. <i>Physical Review E</i> , 2013, 87, 013313.	0.8	14
83	Simulating recrystallization in titanium using the phase field method. <i>IOP Conference Series: Materials Science and Engineering</i> , 2015, 89, 012024.	0.3	14
84	Phase-field simulations of GaN growth by selective area epitaxy from complex mask geometries. <i>Journal of Applied Physics</i> , 2015, 117, .	1.1	14
85	Simulation of the diffusional impedance and application to the characterization of electrodes with complex microstructures. <i>Electrochimica Acta</i> , 2020, 354, 136534.	2.6	14
86	Lowering Ternary Oxide Synthesis Temperatures by Solid-State Cometathesis Reactions. <i>Chemistry of Materials</i> , 2021, 33, 3692-3701.	3.2	14
87	Linear stability analysis for step meandering instabilities with elastic interactions and Ehrlich-Schwoebel barriers. <i>Physical Review E</i> , 2007, 76, 011601.	0.8	13
88	Continuum simulations of the formation of Kirkendall-effect-induced hollow cylinders in a binary substitutional alloy. <i>Acta Materialia</i> , 2009, 57, 5348-5360.	3.8	13
89	Evolution of interfacial curvatures of a bicontinuous structure generated via nonconserved dynamics. <i>Acta Materialia</i> , 2015, 90, 182-193.	3.8	13
90	Charge attachment induced transport – bulk and grain boundary diffusion of potassium in PrMnO <sub>3</sub> . <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 9762-9769.	1.3	13

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91	Current status and outlook of computational materials science education in the US. Modelling and Simulation in Materials Science and Engineering, 2005, 13, R53-R69.	0.8	12
92	The morphology of topologically complex interfaces. Scripta Materialia, 2009, 60, 301-304.	2.6	12
93	Dynamics of two-phase lipid vesicles: effects of mechanical properties on morphology evolution. Soft Matter, 2010, 6, 3462.	1.2	12
94	Ionic and Electronic Transport in Metal Fluoride Conversion Electrodes. ECS Transactions, 2013, 50, 19-25.	0.3	12
95	Simulating complex crystal structures using the phase-field crystal model. Physical Review Materials, 2017, 1, .	0.9	12
96	Conditions for overall planarity in membranes: Applications to multicomponent membranes with lamellar morphology. Europhysics Letters, 2008, 82, 38001.	0.7	11
97	Effects of interleaflet coupling on the morphologies of multicomponent lipid bilayer membranes. Journal of Chemical Physics, 2013, 138, 024909.	1.2	11
98	Model for Anodic Film Growth on Aluminum with Coupled Bulk Transport and Interfacial Reactions. Langmuir, 2014, 30, 5314-5325.	1.6	11
99	A Phase-Field Model and Simulation of Kinetically Asymmetric Ternary Conversion-Reconversion Transformation in Battery Electrodes. Journal of Phase Equilibria and Diffusion, 2016, 37, 86-99.	0.5	11
100	Dynamics of coarsening in multicomponent lipid vesicles with non-uniform mechanical properties. Journal of Chemical Physics, 2014, 140, 144908.	1.2	10
101	Smoothed Boundary Method for simulating bulk and grain boundary transport in complex polycrystalline microstructures. Computational Materials Science, 2016, 121, 14-22.	1.4	10
102	Relative Kinetics of Solid-State Reactions: The Role of Architecture in Controlling Reactivity. Journal of the American Chemical Society, 2022, 144, 11975-11979.	6.6	10
103	Phase-field simulations of GaN/InGaN quantum dot growth by selective area epitaxy. Journal of Crystal Growth, 2012, 361, 57-65.	0.7	9
104	Self-Similarity and the Dynamics of Coarsening in Materials. Scientific Reports, 2018, 8, 17940.	1.6	9
105	Computational Materials Science and Engineering Education: An Updated Survey of Trends and Needs. Jom, 2018, 70, 1644-1651.	0.9	9
106	Thermodynamic relationships for homogeneous crystalline and liquid phases in the phase-field crystal model. Computational Materials Science, 2017, 135, 205-213.	1.4	8
107	Simulation of coarsening in two-phase systems with dissimilar mobilities. Computational Materials Science, 2020, 173, 109418.	1.4	8
108	Towards the Validation of a Phase Field Model for Ni Coarsening in Solid Oxide Cells. Acta Materialia, 2021, 212, 116887.	3.8	8

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109	Effect of transport mechanism on the coarsening of bicontinuous structures: A comparison between bulk and surface diffusion. <i>Physical Review Materials</i> , 2020, 4, .	0.9	8
110	Origins of ion irradiation-induced Ga nanoparticle motion on GaAs surfaces. <i>Applied Physics Letters</i> , 2013, 103, .	1.5	7
111	Origin of broad luminescence from site-controlled InGaN nanodots fabricated by selective area epitaxy. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2014, 211, 531-535.	0.8	7
112	Simulations of Anodic Nanopore Growth Using the Smoothed Boundary and Level Set Methods. <i>Journal of Physical Chemistry C</i> , 2016, 120, 2419-2431.	1.5	7
113	The effect of surface-bulk potential difference on the kinetics of intercalation in core-shell active cathode particles. <i>Journal of Power Sources</i> , 2018, 382, 30-37.	4.0	7
114	Phase Field Modeling of Microstructural Evolution. , 2018, , 67-87.		7
115	Sensitivity analysis of a phase field model for static recrystallization of deformed microstructures. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2020, 28, 065002.	0.8	7
116	Grain boundary formation through particle detachment during coarsening of nanoporous metals. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	7
117	Three-Dimensional Analysis of Solid Oxide Fuel Cells, Using Focused Ion Beam " Scanning Electron Microscopy. <i>Microscopy and Microanalysis</i> , 2007, 13, .	0.2	6
118	Advancing quantitative description of porosity in autogenous laser-welds of 304L stainless steel. <i>Integrating Materials and Manufacturing Innovation</i> , 2014, 3, 141-157.	1.2	6
119	Processing-Dependent Microstructure of $\text{AgCl}/\text{CsAgCl}_2$ Eutectic Photonic Crystals. <i>Advanced Optical Materials</i> , 2018, 6, 1701316.	3.6	6
120	Channel size distribution of complex three-dimensional microstructures calculated from the topological characterization of isodistance structures. <i>Acta Materialia</i> , 2012, 60, 2509-2517.	3.8	5
121	Performance Variability and Degradation in Porous $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ Electrodes. <i>Journal of the Electrochemical Society</i> , 2014, 161, F561-F568.	1.3	5
122	Simulation of the Electrochemical Impedance in a Three-Dimensional, Complex Microstructure of Solid Oxide Fuel Cell Cathode and Its Application in the Microstructure Characterization. <i>Frontiers in Chemistry</i> , 2021, 9, 627699.	1.8	5
123	Stability of strained thin films with interface misfit dislocations: A multiscale computational study. <i>Thin Solid Films</i> , 2010, 519, 809-817.	0.8	4
124	Control of lamellar eutectic orientation via template-directed solidification. <i>Acta Materialia</i> , 2019, 166, 715-722.	3.8	3
125	<i>In situ</i> temperature profile measurements with high-energy X-rays as a probe of optical floating zone crystal growth environment. <i>Journal of Applied Crystallography</i> , 2020, 53, 982-990.	1.9	3
126	Enabling the electrochemical simulation of Li-ion battery electrodes with anisotropic tortuosity in COMSOL Multiphysics. <i>MethodsX</i> , 2021, 8, 101425.	0.7	3



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127	Automated extraction of physical parameters from experimentally obtained thermal profiles using a machine learning approach. <i>Computational Materials Science</i> , 2021, 194, 110459.	1.4	3
128	Thin-Film Paradigm to Probe Interfacial Diffusion during Solid-State Metathesis Reactions. <i>Chemistry of Materials</i> , 2022, 34, 6279-6287.	3.2	3
129	Anomalous strain-energy-driven macroscale translation of grains during nonisothermal annealing. <i>Physical Review Materials</i> , 2021, 5, .	0.9	2
130	Anodic Oxide Nanostructures and Their Applications in Energy Generation and Storage. <i>ACS Symposium Series</i> , 2015, , 19-39.	0.5	1
131	Sample environment effects on synchrotron-measured temperature profiles in an approximant of optical floating zone crystal growth. <i>Journal of Crystal Growth</i> , 2021, 574, 126331.	0.7	1
132	The Mean and Gaussian Curvature of Systems Undergoing Coarsening: Experiment and Theory. <i>Microscopy and Microanalysis</i> , 2004, 10, 74-75.	0.2	0
133	Simulations of the Morphological Evolution of Lipid Bilayer Membranes Using a Phase-Field Method. <i>Biophysical Journal</i> , 2009, 96, 354a-355a.	0.2	0
134	Applying for computational time on NSF's TeraGrid—the world's largest cyberinfrastructure supporting open research. <i>Jom</i> , 2010, 62, 17-18.	0.9	0
135	Phase-Field Modeling and Simulations of Lipid Membranes Coupling Composition with Membrane Mechanical Properties. <i>Biophysical Journal</i> , 2010, 98, 281a.	0.2	0
136	Photonic Crystals: Template-Directed Directionally Solidified 3D Mesostructured AgCl-KCl Eutectic Photonic Crystals ( <i>Adv. Mater.</i> 31/2015). <i>Advanced Materials</i> , 2015, 27, 4550-4550.	11.1	0
137	Rate-dependent Reversal of Lithium Concentration During Intercalation into $\text{Li}_x\text{FePO}_4$ Nanoparticles. <i>Microscopy and Microanalysis</i> , 2018, 24, 1482-1483.	0.2	0