John Gregoire

List of Publications by Year
in descending order

139	5,997	81900 39	85541 71
papers	citations	h-index	g-index

148	148	148	7047
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Lithium-Assisted Plastic Deformation of Silicon Electrodes in Lithium-Ion Batteries: A First-Principles Theoretical Study. Nano Letters, 2011, 11, 2962-2967.	9.1	301
2	The Evolution of the Polycrystalline Copper Surface, First to Cu(111) and Then to Cu(100), at a Fixed CO₂RR Potential: A Study by <i>Operando</i> EC-STM. Langmuir, 2014, 30, 15053-15056.	3.5	245
3	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	2.8	236
4	Fulfilling the promise of the materials genome initiative with high-throughput experimental methodologies. Applied Physics Reviews, 2017, 4, .	11.3	224
5	Inverse Design of Solid-State Materials via a Continuous Representation. Matter, 2019, 1, 1370-1384.	10.0	198
6	Electrochemical Stability of Metastable Materials. Chemistry of Materials, 2017, 29, 10159-10167.	6.7	168
7	Discovering Ce-rich oxygen evolution catalysts, from high throughput screening to water electrolysis. Energy and Environmental Science, 2014, 7, 682-688.	30.8	165
8	Solar fuels photoanode materials discovery by integrating high-throughput theory and experiment. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3040-3043.	7.1	157
9	An Operando Investigation of (Niâ€“Feâ€“Coâ€“Ce)O_{<i>x</i>} System as Highly Efficient Electrocatalyst for Oxygen Evolution Reaction. ACS Catalysis, 2017, 7, 1248-1258.	11.2	156
10	Analysis of the limitations in the oxygen reduction activity of transition metal oxide surfaces. Nature Catalysis, 2021, 4, 463-468.	34.4	156
11	Autonomous experimentation systems for materials development: A community perspective. Matter, 2021, 4, 2702-2726.	10.0	143
12	Robust and synthesizable photocatalysts for CO2 reduction: a data-driven materials discovery. Nature Communications, 2019, 10, 443.	12.8	125
13	High-throughput, combinatorial synthesis of multimetallic nanoclusters. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 6316-6322.	7.1	119
14	High Throughput Light Absorber Discovery, Part 1: An Algorithm for Automated Tauc Analysis. ACS Combinatorial Science, 2016, 18, 673-681.	3.8	118
15	Progress and prospects for accelerating materials science with automated and autonomous workflows. Chemical Science, 2019, 10, 9640-9649.	7.4	114
16	Scanning droplet cell for high throughput electrochemical and photoelectrochemical measurements. Review of Scientific Instruments, 2013, 84, 024102.	1.3	110
17	Rutile Alloys in the Mnâ€“Sbâ€“O System Stabilize Mn³⁺ To Enable Oxygen Evolution in Strong Acid. ACS Catalysis, 2018, 8, 10938-10948.	11.2	97
18	Perspective: Compositionâ€“structureâ€“property mapping in high-throughput experiments: Turning data into knowledge. APL Materials, 2016, 4, .	5.1	87

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19	Machine learning of optical properties of materials â€“ predicting spectra from images and images from spectra. Chemical Science, 2019, 10, 47-55.	7.4	86
20	Multiphase Nanostructure of a Quinary Metal Oxide Electrocatalyst Reveals a New Direction for OER Electrocatalyst Design. Advanced Energy Materials, 2015, 5, 1402307.	19.5	85
21	Benchmarking the acceleration of materials discovery by sequential learning. Chemical Science, 2020, 11, 2696-2706.	7.4	83
22	High Throughput Discovery of Solar Fuels Photoanodes in the CuOâ€“V₂O₅ System. Advanced Energy Materials, 2015, 5, 1500968.	19.5	82
23	Highâ€Throughput Mapping of the Electrochemical Properties of (Niâ€Feâ€Coâ€Ce)O_{<i>x</i>} Oxygenâ€Evolution Catalysts. ChemElectroChem, 2014, 1, 524-528.	3.4	71
24	High-Throughput Bubble Screening Method for Combinatorial Discovery of Electrocatalysts for Water Splitting. ACS Combinatorial Science, 2014, 16, 47-52.	3.8	70
25	Mn₂V₂O₇: An Earth Abundant Light Absorber for Solar Water Splitting. Advanced Energy Materials, 2015, 5, 1401840.	19.5	61
26	Development of solar fuels photoanodes through combinatorial integration of Niâ€“Laâ€“Coâ€“Ce oxide catalysts on BiVO₄. Energy and Environmental Science, 2016, 9, 565-580.	30.8	61
27	Automated Phase Mapping with AgileFD and its Application to Light Absorber Discovery in the Vâ€“Mnâ€“Nb Oxide System. ACS Combinatorial Science, 2017, 19, 37-46.	3.8	61
28	Artificial intelligence for materials discovery. MRS Bulletin, 2019, 44, 538-544.	3.5	60
29	Analyzing machine learning models to accelerate generation of fundamental materials insights. Npj Computational Materials, 2019, 5, .	8.7	60
30	The 2022 solar fuels roadmap. Journal Physics D: Applied Physics, 2022, 55, 323003.	2.8	58
31	Ethanol-Promoted High-Yield Growth of Few-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 6389-6395.	3.1	56
32	High-throughput synchrotron X-ray diffraction forÂcombinatorial phase mapping. Journal of Synchrotron Radiation, 2014, 21, 1262-1268.	2.4	56
33	Stability and self-passivation of copper vanadate photoanodes under chemical, electrochemical, and photoelectrochemical operation. Physical Chemistry Chemical Physics, 2016, 18, 9349-9352.	2.8	56
34	Solar fuel photoanodes prepared by inkjet printing of copper vanadates. Journal of Materials Chemistry A, 2016, 4, 7483-7494.	10.3	56
35	A wavelet transform algorithm for peak detection and application to powder x-ray diffraction data. Review of Scientific Instruments, 2011, 82, 015105.	1.3	54
36	High-Throughput Screening for Acid-Stable Oxygen Evolution Electrocatalysts in the (Mnâ€“Coâ€“Taâ€“Sb)O x Composition Space. Electrocatalysis, 2015, 6, 229-236.	3.0	53

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37	Combined Catalysis and Optical Screening for High Throughput Discovery of Solar Fuels Catalysts. Journal of the Electrochemical Society, 2013, 160, F337-F342.	2.9	50
38	Combining combinatorial nanocalorimetry and X-ray diffraction techniques to study the effects of composition and quench rate on Auâ€“Cuâ€“Si metallic glasses. Scripta Materialia, 2012, 66, 178-181.	5.2	49
39	Computational sustainability. Communications of the ACM, 2019, 62, 56-65.	4.5	49
40	Bimetallic effects on Zn-Cu electrocatalysts enhance activity and selectivity for the conversion of CO2 to CO. Chem Catalysis, 2021, 1, 663-680.	6.1	42
41	Designing a Znâ€“Ag Catalyst Matrix and Electrolyzer System for CO₂ Conversion to CO and Beyond. Advanced Materials, 2022, 34, e2103963.	21.0	41
42	Tracking materials science data lineage to manage millions of materials experiments and analyses. Npj Computational Materials, 2019, 5, .	8.7	40
43	High energy x-ray diffraction/x-ray fluorescence spectroscopy for high-throughput analysis of composition spread thin films. Review of Scientific Instruments, 2009, 80, 123905.	1.3	39
44	A scanning AC calorimetry technique for the analysis of nano-scale quantities of materials. Review of Scientific Instruments, 2012, 83, 114901.	1.3	39
45	High mobility single crystalline ScN and single-orientation epitaxial YN on sapphire via magnetron sputtering. Journal of Applied Physics, 2008, 104, .	2.5	37
46	High-Throughput Evaluation of Dealloyed Ptâ€“Zn Composition-Spread Thin Film for Methanol-Oxidation Catalysis. Journal of the Electrochemical Society, 2009, 156, B160.	2.9	37
47	Electrocatalytic Reduction of Nitrogen and Carbon Dioxide to Chemical Fuels: Challenges and Opportunities for a Solar Fuel Device. Journal of Photochemistry and Photobiology B: Biology, 2015, 152, 47-57.	3.8	37
48	Generating Information-Rich High-Throughput Experimental Materials Genomes using Functional Clustering via Multitree Genetic Programming and Information Theory. ACS Combinatorial Science, 2015, 17, 224-233.	3.8	37
49	Scanning AC nanocalorimetry combined with <i>in-situ</i> x-ray diffraction. Journal of Applied Physics, 2013, 113, .	2.5	36
50	Discovery of Manganese-Based Solar Fuel Photoanodes via Integration of Electronic Structure Calculations, Pourbaix Stability Modeling, and High-Throughput Experiments. ACS Energy Letters, 2017, 2, 2307-2312.	17.4	36
51	Discovery of Feâ€“Ce Oxide/BiVO₄ Photoanodes through Combinatorial Exploration of Niâ€“Feâ€“Coâ€“Ce Oxide Coatings. ACS Applied Materials & Interfaces, 2016, 8, 23696-23705.	8.0	35
52	<i>In-situ</i> X-ray diffraction combined with scanning AC nanocalorimetry applied to a Fe0.84Ni0.16 thin-film sample. Applied Physics Letters, 2013, 102, 201902.	3.3	33
53	Getter sputtering system for high-throughput fabrication of composition spreads. Review of Scientific Instruments, 2007, 78, 072212.	1.3	31
54	High-throughput on-the-fly scanning ultraviolet-visible dual-sphere spectrometer. Review of Scientific Instruments, 2015, 86, 013904.	1.3	31

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55	Materials representation and transfer learning for multi-property prediction. Applied Physics Reviews, 2021, 8, .	11.3	31
56	Solidification of Au-Cu-Si alloys investigated by a combinatorial approach. Journal of Applied Physics, 2012, 111, .	2.5	30
57	Combinatorial thin film composition mapping using three dimensional deposition profiles. Review of Scientific Instruments, 2015, 86, 033904.	1.3	30
58	Successes and Opportunities for Discovery of Metal Oxide Photoanodes for Solar Fuels Generators. ACS Energy Letters, 2020, 5, 1413-1421.	17.4	30
59	Discovery of New Oxygen Evolution Reaction Electrocatalysts by Combinatorial Investigation of the Niâ€"Laâ€"Coâ€"Ce Oxide Composition Space. ChemElectroChem, 2014, 1, 1613-1617.	3.4	29
60	Automating crystal-structure phase mapping by combining deep learning with constraint reasoning. Nature Machine Intelligence, 2021, 3, 812-822.	16.0	29
61	The case for data science in experimental chemistry: examples and recommendations. Nature Reviews Chemistry, 2022, 6, 357-370.	30.2	29
62	Structural, electronic and optical properties of (Sc,Y)N solid solutions. Thin Solid Films, 2009, 517, 1607-1609.	1.8	28
63	Improved Fuel Cell Oxidation Catalysis in Pt_{1â^'<i>x</i>}Ta_{<i>x</i>}. Chemistry of Materials, 2010, 22, 1080-1087.	6.7	28
64	Synthesis of Ptâ^'Moâ^'N Thin Film and Catalytic Activity for Fuel Cells. Chemistry of Materials, 2010, 22, 3451-3456.	6.7	28
65	Interface engineering for light-driven water oxidation: unravelling the passivating and catalytic mechanism in BiVO₄ overlayers. Sustainable Energy and Fuels, 2019, 3, 127-135.	4.9	28
66	Fermi Level Engineering of Passivation and Electron Transport Materials for pâ€Type CuBi 2 O 4 Employing a Highâ€Throughput Methodology. Advanced Functional Materials, 2020, 30, 2000948.	14.9	28
67	JCAP Research on Solar Fuel Production at Light Sources. Synchrotron Radiation News, 2014, 27, 14-17.	0.8	26
68	Constraint Reasoning and Kernel Clustering for Pattern Decomposition with Scaling. Lecture Notes in Computer Science, 2011, , 508-522.	1.3	26
69	Breaking Scaling Relationships in CO₂ Reduction on Copper Alloys with Organic Additives. ACS Central Science, 2021, 7, 1756-1762.	11.3	26
70	Density of states prediction for materials discovery via contrastive learning from probabilistic embeddings. Nature Communications, 2022, 13, 949.	12.8	26
71	Autonomous materials synthesis via hierarchical active learning of nonequilibrium phase diagrams. Science Advances, 2021, 7, eabg4930.	10.3	26
72	Mapping Quantum Yield for (Feâ€"Znâ€"Snâ€"Ti)Ox Photoabsorbers Using a High Throughput Photoelectrochemical Screening System. ACS Combinatorial Science, 2014, 16, 120-127.	3.8	23

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73	Enabling Modular Autonomous Feedbackâ€Loops in Materials Science through Hierarchical Experimental Laboratory Automation and Orchestration. Advanced Materials Interfaces, 2022, 9, 2101987.	3.7	23
74	Application of in-situ nano-scanning calorimetry and X-ray diffraction to characterize Niâ€“Tiâ€“Hf high-temperature shape memory alloys. Thermochimica Acta, 2015, 603, 53-62.	2.7	22
75	Electrochemical surface science twenty years later: Expeditions into the electrocatalysis of reactions at the core of artificial photosynthesis. Surface Science, 2015, 631, 285-294.	1.9	22
76	CRYSTAL: a multi-agent AI system for automated mapping of materialsâ€™ crystal structures. MRS Communications, 2019, 9, 600-608.	1.8	22
77	Functional mapping reveals mechanistic clusters for OER catalysis across (Cuâ€“Mnâ€“Taâ€“Coâ€“Snâ€“Fe)O_x composition and pH space. Materials Horizons, 2019, 6, 1251-1258.	12.2	22
78	Combinatorial alloying improves bismuth vanadate photoanodes <i>via</i> reduced monoclinic distortion. Energy and Environmental Science, 2018, 11, 2444-2457.	30.8	21
79	Multi-component background learning automates signal detection for spectroscopic data. Npj Computational Materials, 2019, 5, .	8.7	21
80	Discovery of complex oxides via automated experiments and data science. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	21
81	Stability and Activity of Cobalt Antimonate for Oxygen Reduction in Strong Acid. ACS Energy Letters, 2022, 7, 993-1000.	17.4	21
82	Bi-Containing n-FeWO4 Thin Films Provide the Largest Photovoltage and Highest Stability for a Sub-2 eV Band Gap Photoanode. ACS Energy Letters, 2018, 3, 2769-2774.	17.4	20
83	Ptâˆ’Cd and Ptâˆ’Hg Phases As High Activity Catalysts for Methanol and Formic Acid Oxidation. Journal of Physical Chemistry C, 2010, 114, 12545-12553.	3.1	19
84	Statistical Analysis and Interpolation of Compositional Data in Materials Science. ACS Combinatorial Science, 2015, 17, 130-136.	3.8	19
85	The role of the CeO₂/BiVO₄ interface in optimized Feâ€“Ce oxide coatings for solar fuels photoanodes. Journal of Materials Chemistry A, 2016, 4, 14356-14363.	10.3	19
86	High Throughput Light Absorber Discovery, Part 2: Establishing Structureâ€“Band Gap Energy Relationships. ACS Combinatorial Science, 2016, 18, 682-688.	3.8	19
87	The Materials Research Platform: Defining the Requirements from User Stories. Matter, 2019, 1, 1433-1438.	10.0	19
88	Unveiling new stable manganese based photoanode materials <i>via</i> theoretical high-throughput screening and experiments. Chemical Communications, 2019, 55, 13418-13421.	4.1	18
89	Discovery and Characterization of a Pourbaix-Stable, 1.8 eV Direct Gap Bismuth Manganate Photoanode. Chemistry of Materials, 2017, 29, 10027-10036.	6.7	17
90	Phaseâ€Mapper: Accelerating Materials Discovery with AI. AI Magazine, 2018, 39, 15-26.	1.6	17

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91	Overcoming Hurdles in Oxygen Evolution Catalyst Discovery via Codesign. Chemistry of Materials, 2022, 34, 899-910.	6.7	17
92	Resputtering phenomena and determination of composition in codeposited films. Physical Review B, 2007, 76, .	3.2	16
93	High Throughput Thin Film Pt-M Alloys for Fuel Electrooxidation: Low Concentrations of M (M = Sn,) Tj ETQq1 1 0.784314 rgBT /Overlo 159, F880-F887.	2.9	16
94	Identification of optimal solar fuel electrocatalysts via high throughput in situ optical measurements. Journal of Materials Research, 2015, 30, 442-450.	2.6	16
95	Quaternary Oxide Photoanode Discovery Improves the Spectral Response and Photovoltage of Copper Vanadates. Matter, 2020, 3, 1614-1630.	10.0	16
96	Combinatorial Discovery of Lanthanumâ€"Tantalum Oxynitride Solar Light Absorbers with Dilute Nitrogen for Solar Fuel Applications. ACS Combinatorial Science, 2018, 20, 26-34.	3.8	15
97	Scanning Electrochemical Flow Cell with Online Mass Spectroscopy for Accelerated Screening of Carbon Dioxide Reduction Electrocatalysts. ACS Combinatorial Science, 2019, 21, 692-704.	3.8	15
98	Multi-modal optimization of bismuth vanadate photoanodes <i>via</i> combinatorial alloying and hydrogen processing. Chemical Communications, 2019, 55, 489-492.	4.1	15
99	Synthesis, optical imaging, and absorption spectroscopy data for 179072 metal oxides. Scientific Data, 2019, 6, 9.	5.3	14
100	Combinatorial screening yields discovery of 29 metal oxide photoanodes for solar fuel generation. Journal of Materials Chemistry A, 2020, 8, 4239-4243.	10.3	13
101	Combining reactive sputtering and rapid thermal processing for synthesis and discovery of metal oxynitrides. Journal of Materials Research, 2015, 30, 2928-2933.	2.6	12
102	Colorimetric Screening for High-Throughput Discovery of Light Absorbers. ACS Combinatorial Science, 2015, 17, 176-181.	3.8	12
103	Parallel Electrochemical Treatment System and Application for Identifying Acid-Stable Oxygen Evolution Electrocatalysts. ACS Combinatorial Science, 2015, 17, 71-75.	3.8	12
104	High-Throughput Measurement of Ionic Conductivity in Composition-Spread Thin Films. ACS Combinatorial Science, 2013, 15, 273-277.	3.8	11
105	Reactor design and integration with product detection to accelerate screening of electrocatalysts for carbon dioxide reduction. Review of Scientific Instruments, 2018, 89, 124102.	1.3	11
106	The sensitivity of Cu for electrochemical carbon dioxide reduction to hydrocarbons as revealed by high throughput experiments. Journal of Materials Chemistry A, 2019, 7, 26785-26790.	10.3	10
107	Enhanced Bulk Transport in Copper Vanadate Photoanodes Identified by Combinatorial Alloying. Matter, 2020, 3, 1601-1613.	10.0	8
108	Computational sustainability meets materials science. Nature Reviews Materials, 2021, 6, 645-647.	48.7	8

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109	Band Edge Energy Tuning through Electronic Character Hybridization in Ternary Metal Vanadates. Chemistry of Materials, 2021, 33, 7242-7253.	6.7	7
110	High Throughput Discovery of Complex Metal Oxide Electrocatalysts for the Oxygen Reduction Reaction. Electrocatalysis, 2022, 13, 1-10.	3.0	7
111	A model for calculating resputter rates in codeposition. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2008, 26, 1030-1036.	2.1	6
112	Cosputtered composition-spread reproducibility established by high-throughput x-ray fluorescence. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2010, 28, 1279-1280.	2.1	6
113	Molecular Coatings Improve the Selectivity and Durability of CO₂ Reduction Chalcogenide Photocathodes. ACS Energy Letters, 2022, 7, 1195-1201.	17.4	6
114	Addressing solar photochemistry durability with an amorphous nickel antimonate photoanode. Cell Reports Physical Science, 2022, 3, 100959.	5.6	6
115	General counting formulae for factorized time correlation diagram analysis. Physica A: Statistical Mechanics and Its Applications, 2003, 320, 1-10.	2.6	5
116	An upgraded high-velocity dust particle accelerator at Concordia College in Moorhead, Minnesota. International Journal of Impact Engineering, 2006, 33, 402-409.	5.0	5
117	Phase Behavior of Pseudobinary Precious Metalâˆ'Carbide Systems. Journal of Physical Chemistry C, 2010, 114, 21664-21671.	3.1	5
118	High Throughput X-ray Diffraction Analysis of Combinatorial Polycrystalline Thin Film Libraries. Analytical Chemistry, 2010, 82, 4564-4569.	6.5	5
119	Bi Alloying into Rare Earth Double Perovskites Enhances Synthesizability and Visible Light Absorption. ACS Combinatorial Science, 2020, 22, 895-901.	3.8	5
120	Relaxation Methods for Constrained Matrix Factorization Problems: Solving the Phase Mapping Problem in Materials Discovery. Lecture Notes in Computer Science, 2017, , 104-112.	1.3	5
121	Advanced and In Situ Analytical Methods for Solar Fuel Materials. Topics in Current Chemistry, 2015, 371, 253-324.	4.0	4
122	An Efficient Relaxed Projection Method for Constrained Non-negative Matrix Factorization with Application to the Phase-Mapping Problem in Materials Science. Lecture Notes in Computer Science, 2018, , 52-62.	1.3	4
123	Optical Identification of Materials Transformations in Oxide Thin Films. ACS Combinatorial Science, 2020, 22, 887-894.	3.8	4
124	Combined Catalysis and Optical Screening for High Throughput Discovery of Solar Fuels Catalysts. ECS Transactions, 2013, 50, 9-20.	0.5	3
125	Imitation Refinement for X-ray Diffraction Signal Processing. , 2019, , .		3
126	Materials structureâ€"property factorization for identification of synergistic phase interactions in complex solar fuels photoanodes. Npj Computational Materials, 2022, 8, .	8.7	3

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127	High throughput discovery of enhanced visible photoactivity in Feâ€"Cr vanadate solar fuels photoanodes. JPhys Energy, 2022, 4, 044001.	5.3	3
128	High Throughput Combinatorial Experimentation + Informatics = Combinatorial Science. Springer Series in Materials Science, 2016, , 271-300.	0.6	2
129	Alkaline-stable nickel manganese oxides with ideal band gap for solar fuel photoanodes. Chemical Communications, 2018, 54, 4625-4628.	4.1	2
130	Balancing Surface Passivation and Catalysis with Integrated BiVO4/(Feâ€"Ce)Ox Photoanodes in pH 9 Borate Electrolyte. ACS Applied Energy Materials, 2018, , .	5.1	2
131	Enabling Solar Fuels Technology With High Throughput Experimentation. Materials Research Society Symposia Proceedings, 2014, 1654, 1.	0.1	1
132	Unexpected Transitions Yield Interesting Science and High-Performance Materials. Matter, 2019, 1, 790-791.	10.0	1
133	Combinatorial Synthesis of Oxysulfides in the Lanthanumâ€"Bismuth-Copper System. ACS Combinatorial Science, 2020, 22, 319-326.	3.8	1
134	High Throughput Evaluation of Multi-Element, Multi-Functional Coatings for Improved Photoanodes and Photocathodes. ECS Meeting Abstracts, 2021, MA2021-01, 1267-1267.	0.0	0
135	Chapter 9. High Throughput Experimentation for the Discovery of Water Splitting Materials. RSC Energy and Environment Series, 2018, , 305-340.	0.5	0
136	(Invited) Accelerated Discovery for Solar Fuels. ECS Meeting Abstracts, 2019, , .	0.0	0
137	(Invited) High Throughput Synthesis As an Enabling Capability for Materials and Interface Discovery. ECS Meeting Abstracts, 2019, , .	0.0	0
138	Accelerated Screening for Carbon Dioxide Reduction Electrocatalysts and Implications for Reactor Design. ECS Meeting Abstracts, 2019, , .	0.0	0
139	(Invited) Integrating High Throughput Synthesis with Characterization and Computation for Accelerated Discovery of Energy Conversion Materials. ECS Meeting Abstracts, 2021, MA2021-02, 1346-1346.	0.0	0