John Gregoire

List of Publications by Year
in descending order

139 papers	5,997 citations	93792 39 h-index	97045 71 g-index
148 all docs	148 docs citations	148 times ranked	8221 citing authors

#	Article	IF	Citations
1	Designing a Znâ€“Ag Catalyst Matrix and Electrolyzer System for CO₂ Conversion to CO and Beyond. Advanced Materials, 2022, 34, e2103963.	11.1	41
2	High Throughput Discovery of Complex Metal Oxide Electrocatalysts for the Oxygen Reduction Reaction. Electrocatalysis, 2022, 13, 1-10.	1.5	7
3	Enabling Modular Autonomous Feedbackâ€Łoops in Materials Science through Hierarchical Experimental Laboratory Automation and Orchestration. Advanced Materials Interfaces, 2022, 9, 2101987.	1.9	23
4	Overcoming Hurdles in Oxygen Evolution Catalyst Discovery via Codesign. Chemistry of Materials, 2022, 34, 899-910.	3.2	17
5	Stability and Activity of Cobalt Antimonate for Oxygen Reduction in Strong Acid. ACS Energy Letters, 2022, 7, 993-1000.	8.8	21
6	Density of states prediction for materials discovery via contrastive learning from probabilistic embeddings. Nature Communications, 2022, 13, 949.	5.8	26
7	Molecular Coatings Improve the Selectivity and Durability of CO₂ Reduction Chalcogenide Photocathodes. ACS Energy Letters, 2022, 7, 1195-1201.	8.8	6
8	Materials structureâ€“property factorization for identification of synergistic phase interactions in complex solar fuels photoanodes. Npj Computational Materials, 2022, 8, .	3.5	3
9	The case for data science in experimental chemistry: examples and recommendations. Nature Reviews Chemistry, 2022, 6, 357-370.	13.8	29
10	The 2022 solar fuels roadmap. Journal Physics D: Applied Physics, 2022, 55, 323003.	1.3	58
11	Addressing solar photochemistry durability with an amorphous nickel antimonate photoanode. Cell Reports Physical Science, 2022, 3, 100959.	2.8	6
12	High throughput discovery of enhanced visible photoactivity in Feâ€“Cr vanadate solar fuels photoanodes. JPhys Energy, 2022, 4, 044001.	2.3	3
13	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
14	Analysis of the limitations in the oxygen reduction activity of transition metal oxide surfaces. Nature Catalysis, 2021, 4, 463-468.	16.1	156
15	Materials representation and transfer learning for multi-property prediction. Applied Physics Reviews, 2021, 8, .	5.5	31
16	Computational sustainability meets materials science. Nature Reviews Materials, 2021, 6, 645-647.	23.3	8
17	Bimetallic effects on Zn-Cu electrocatalysts enhance activity and selectivity for the conversion of CO2 to CO. Chem Catalysis, 2021, 1, 663-680.	2.9	42
18	Band Edge Energy Tuning through Electronic Character Hybridization in Ternary Metal Vanadates. Chemistry of Materials, 2021, 33, 7242-7253.	3.2	7

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19	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, .	3.3	21
20	Automating crystal-structure phase mapping by combining deep learning with constraint reasoning. Nature Machine Intelligence, 2021, 3, 812-822.	8.3	29
21	Autonomous experimentation systems for materials development: A community perspective. Matter, 2021, 4, 2702-2726.	5.0	143
22	Breaking Scaling Relationships in CO₂ Reduction on Copper Alloys with Organic Additives. ACS Central Science, 2021, 7, 1756-1762.	5.3	26
23	(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
24	Autonomous materials synthesis via hierarchical active learning of nonequilibrium phase diagrams. Science Advances, 2021, 7, eabg4930.	4.7	26
25	Quaternary Oxide Photoanode Discovery Improves the Spectral Response and Photovoltage of Copper Vanadates. Matter, 2020, 3, 1614-1630.	5.0	16
26	Enhanced Bulk Transport in Copper Vanadate Photoanodes Identified by Combinatorial Alloying. Matter, 2020, 3, 1601-1613.	5.0	8
27	Bi Alloying into Rare Earth Double Perovskites Enhances Synthesizability and Visible Light Absorption. ACS Combinatorial Science, 2020, 22, 895-901.	3.8	5
28	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.	7.8	28
29	Combinatorial Synthesis of Oxysulfides in the Lanthanumâ€“Bismuth-Copper System. ACS Combinatorial Science, 2020, 22, 319-326.	3.8	1
30	Successes and Opportunities for Discovery of Metal Oxide Photoanodes for Solar Fuels Generators. ACS Energy Letters, 2020, 5, 1413-1421.	8.8	30
31	Combinatorial screening yields discovery of 29 metal oxide photoanodes for solar fuel generation. Journal of Materials Chemistry A, 2020, 8, 4239-4243.	5.2	13
32	Benchmarking the acceleration of materials discovery by sequential learning. Chemical Science, 2020, 11, 2696-2706.	3.7	83
33	High-throughput, combinatorial synthesis of multimetallic nanoclusters. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 6316-6322.	3.3	119
34	Optical Identification of Materials Transformations in Oxide Thin Films. ACS Combinatorial Science, 2020, 22, 887-894.	3.8	4
35	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236
36	Imitation Refinement for X-ray Diffraction Signal Processing. , 2019, , .		3

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37	Artificial intelligence for materials discovery. MRS Bulletin, 2019, 44, 538-544.	1.7	60
38	Multi-component background learning automates signal detection for spectroscopic data. Npj Computational Materials, 2019, 5, .	3.5	21
39	Tracking materials science data lineage to manage millions of materials experiments and analyses. Npj Computational Materials, 2019, 5, .	3.5	40
40	Unexpected Transitions Yield Interesting Science and High-Performance Materials. Matter, 2019, 1, 790-791.	5.0	1
41	Computational sustainability. Communications of the ACM, 2019, 62, 56-65.	3.3	49
42	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
43	Inverse Design of Solid-State Materials via a Continuous Representation. Matter, 2019, 1, 1370-1384.	5.0	198
44	Interface engineering for light-driven water oxidation: unravelling the passivating and catalytic mechanism in BiVO₄ overlayers. Sustainable Energy and Fuels, 2019, 3, 127-135.	2.5	28
45	Multi-modal optimization of bismuth vanadate photoanodes <i>via</i> combinatorial alloying and hydrogen processing. Chemical Communications, 2019, 55, 489-492.	2.2	15
46	Machine learning of optical properties of materials â€“ predicting spectra from images and images from spectra. Chemical Science, 2019, 10, 47-55.	3.7	86
47	Robust and synthesizable photocatalysts for CO2 reduction: a data-driven materials discovery. Nature Communications, 2019, 10, 443.	5.8	125
48	CRYSTAL: a multi-agent AI system for automated mapping of materialsâ€™ crystal structures. MRS Communications, 2019, 9, 600-608.	0.8	22
49	Analyzing machine learning models to accelerate generation of fundamental materials insights. Npj Computational Materials, 2019, 5, .	3.5	60
50	Synthesis, optical imaging, and absorption spectroscopy data for 179072 metal oxides. Scientific Data, 2019, 6, 9.	2.4	14
51	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.	6.4	22
52	Unveiling new stable manganese based photoanode materials <i>via</i> theoretical high-throughput screening and experiments. Chemical Communications, 2019, 55, 13418-13421.	2.2	18
53	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.	5.2	10
54	The Materials Research Platform: Defining the Requirements from User Stories. Matter, 2019, 1, 1433-1438.	5.0	19

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55	Progress and prospects for accelerating materials science with automated and autonomous workflows. Chemical Science, 2019, 10, 9640-9649.	3.7	114
56	(Invited) Accelerated Discovery for Solar Fuels. ECS Meeting Abstracts, 2019, , .	0.0	0
57	(Invited) High Throughput Synthesis As an Enabling Capability for Materials and Interface Discovery. ECS Meeting Abstracts, 2019, , .	0.0	0
58	Accelerated Screening for Carbon Dioxide Reduction Electrocatalysts and Implications for Reactor Design. ECS Meeting Abstracts, 2019, , .	0.0	0
59	Alkaline-stable nickel manganese oxides with ideal band gap for solar fuel photoanodes. Chemical Communications, 2018, 54, 4625-4628.	2.2	2
60	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
61	Phaseâ€Mapper: Accelerating Materials Discovery with AI. AI Magazine, 2018, 39, 15-26.	1.4	17
62	Reactor design and integration with product detection to accelerate screening of electrocatalysts for carbon dioxide reduction. Review of Scientific Instruments, 2018, 89, 124102.	0.6	11
63	Balancing Surface Passivation and Catalysis with Integrated BiVO4/(Feâ€"Ce)Ox Photoanodes in pH 9 Borate Electrolyte. ACS Applied Energy Materials, 2018, , .	2.5	2
64	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.	8.8	20
65	Rutile Alloys in the Mnâ€"Sbâ€"O System Stabilize Mn³⁺ To Enable Oxygen Evolution in Strong Acid. ACS Catalysis, 2018, 8, 10938-10948.	5.5	97
66	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.	1.0	4
67	Combinatorial alloying improves bismuth vanadate photoanodes <i>via</i> reduced monoclinic distortion. Energy and Environmental Science, 2018, 11, 2444-2457.	15.6	21
68	Chapter 9. High Throughput Experimentation for the Discovery of Water Splitting Materials. RSC Energy and Environment Series, 2018, , 305-340.	0.2	0
69	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.	3.3	157
70	Fulfilling the promise of the materials genome initiative with high-throughput experimental methodologies. Applied Physics Reviews, 2017, 4, .	5.5	224
71	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.	5.5	156
72	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

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73	Electrochemical Stability of Metastable Materials. Chemistry of Materials, 2017, 29, 10159-10167.	3.2	168
74	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.	8.8	36
75	Discovery and Characterization of a Pourbaix-Stable, 1.8 eV Direct Gap Bismuth Manganate Photoanode. Chemistry of Materials, 2017, 29, 10027-10036.	3.2	17
76	Relaxation Methods for Constrained Matrix Factorization Problems: Solving the Phase Mapping Problem in Materials Discovery. Lecture Notes in Computer Science, 2017, , 104-112.	1.0	5
77	Stability and self-passivation of copper vanadate photoanodes under chemical, electrochemical, and photoelectrochemical operation. Physical Chemistry Chemical Physics, 2016, 18, 9349-9352.	1.3	56
78	Solar fuel photoanodes prepared by inkjet printing of copper vanadates. Journal of Materials Chemistry A, 2016, 4, 7483-7494.	5.2	56
79	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.	5.2	19
80	High Throughput Light Absorber Discovery, Part 1: An Algorithm for Automated Tauc Analysis. ACS Combinatorial Science, 2016, 18, 673-681.	3.8	118
81	High Throughput Light Absorber Discovery, Part 2: Establishing Structureâ€“Band Gap Energy Relationships. ACS Combinatorial Science, 2016, 18, 682-688.	3.8	19
82	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.	4.0	35
83	Perspective: Compositionâ€“structureâ€“property mapping in high-throughput experiments: Turning data into knowledge. APL Materials, 2016, 4, .	2.2	87
84	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.	15.6	61
85	High Throughput Combinatorial Experimentation + Informatics = Combinatorial Science. Springer Series in Materials Science, 2016, , 271-300.	0.4	2
86	Combining reactive sputtering and rapid thermal processing for synthesis and discovery of metal oxynitrides. Journal of Materials Research, 2015, 30, 2928-2933.	1.2	12
87	High Throughput Discovery of Solar Fuels Photoanodes in the CuOâ€“V₂O₅ System. Advanced Energy Materials, 2015, 5, 1500968.	10.2	82
88	Identification of optimal solar fuel electrocatalysts via high throughput in situ optical measurements. Journal of Materials Research, 2015, 30, 442-450.	1.2	16
89	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.	1.7	37
90	Statistical Analysis and Interpolation of Compositional Data in Materials Science. ACS Combinatorial Science, 2015, 17, 130-136.	3.8	19

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91	Colorimetric Screening for High-Throughput Discovery of Light Absorbers. ACS Combinatorial Science, 2015, 17, 176-181.	3.8	12
92	Parallel Electrochemical Treatment System and Application for Identifying Acid-Stable Oxygen Evolution Electrocatalysts. ACS Combinatorial Science, 2015, 17, 71-75.	3.8	12
93	Mn₂V₂O₇: An Earth Abundant Light Absorber for Solar Water Splitting. Advanced Energy Materials, 2015, 5, 1401840.	10.2	61
94	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.	1.2	22
95	High-Throughput Screening for Acid-Stable Oxygen Evolution Electrocatalysts in the (Mnâ€“Coâ€“Taâ€“Sb)O x Composition Space. Electrocatalysis, 2015, 6, 229-236.	1.5	53
96	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
97	High-throughput on-the-fly scanning ultraviolet-visible dual-sphere spectrometer. Review of Scientific Instruments, 2015, 86, 013904.	0.6	31
98	Multiphase Nanostructure of a Quinary Metal Oxide Electrocatalyst Reveals a New Direction for OER Electrocatalyst Design. Advanced Energy Materials, 2015, 5, 1402307.	10.2	85
99	Combinatorial thin film composition mapping using three dimensional deposition profiles. Review of Scientific Instruments, 2015, 86, 033904.	0.6	30
100	Advanced and In Situ Analytical Methods for Solar Fuel Materials. Topics in Current Chemistry, 2015, 371, 253-324.	4.0	4
101	Electrochemical surface science twenty years later: Expeditions into the electrocatalysis of reactions at the core of artificial photosynthesis. Surface Science, 2015, 631, 285-294.	0.8	22
102	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.	1.6	245
103	Enabling Solar Fuels Technology With High Throughput Experimentation. Materials Research Society Symposia Proceedings, 2014, 1654, 1.	0.1	1
104	High-throughput synchrotron X-ray diffraction forÂcombinatorial phase mapping. Journal of Synchrotron Radiation, 2014, 21, 1262-1268.	1.0	56
105	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
106	JCAP Research on Solar Fuel Production at Light Sources. Synchrotron Radiation News, 2014, 27, 14-17.	0.2	26
107	Discovering Ce-rich oxygen evolution catalysts, from high throughput screening to water electrolysis. Energy and Environmental Science, 2014, 7, 682-688.	15.6	165
108	Discovery of New Oxygen Evolution Reaction Electrocatalysts by Combinatorial Investigation of the Niâ€“Laâ€“Coâ€“Ce Oxide Composition Space. ChemElectroChem, 2014, 1, 1613-1617.	1.7	29

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109	Highâ€Throughput Mapping of the Electrochemical Properties of (Niâ€Feâ€Coâ€Ce)O_{<i>x</i>} Oxygenâ€Evolution Catalysts. ChemElectroChem, 2014, 1, 524-528.	1.7	71
110	High-Throughput Bubble Screening Method for Combinatorial Discovery of Electrocatalysts for Water Splitting. ACS Combinatorial Science, 2014, 16, 47-52.	3.8	70
111	High-Throughput Measurement of Ionic Conductivity in Composition-Spread Thin Films. ACS Combinatorial Science, 2013, 15, 273-277.	3.8	11
112	Scanning droplet cell for high throughput electrochemical and photoelectrochemical measurements. Review of Scientific Instruments, 2013, 84, 024102.	0.6	110
113	Combined Catalysis and Optical Screening for High Throughput Discovery of Solar Fuels Catalysts. Journal of the Electrochemical Society, 2013, 160, F337-F342.	1.3	50
114	Combined Catalysis and Optical Screening for High Throughput Discovery of Solar Fuels Catalysts. ECS Transactions, 2013, 50, 9-20.	0.3	3
115	<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.	1.5	33
116	Scanning AC nanocalorimetry combined with <i>in-situ</i> x-ray diffraction. Journal of Applied Physics, 2013, 113, .	1.1	36
117	High Throughput Thin Film Pt-M Alloys for Fuel Electrooxidation: Low Concentrations of M (M = Sn,) Tj ETQq1 1 0.784314 rgBT /Overl 159, F880-F887.	1.3	16
118	Solidification of Au-Cu-Si alloys investigated by a combinatorial approach. Journal of Applied Physics, 2012, 111, .	1.1	30
119	A scanning AC calorimetry technique for the analysis of nano-scale quantities of materials. Review of Scientific Instruments, 2012, 83, 114901.	0.6	39
120	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.	2.6	49
121	Lithium-Assisted Plastic Deformation of Silicon Electrodes in Lithium-Ion Batteries: A First-Principles Theoretical Study. Nano Letters, 2011, 11, 2962-2967.	4.5	301
122	A wavelet transform algorithm for peak detection and application to powder x-ray diffraction data. Review of Scientific Instruments, 2011, 82, 015105.	0.6	54
123	Constraint Reasoning and Kernel Clustering for Pattern Decomposition with Scaling. Lecture Notes in Computer Science, 2011, , 508-522.	1.0	26
124	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.	0.9	6
125	Improved Fuel Cell Oxidation Catalysis in Pt_{1â^’<i>x</i>}Ta_{<i>x</i>}. Chemistry of Materials, 2010, 22, 1080-1087.	3.2	28
126	Synthesis of Ptâ^’Moâ^’N Thin Film and Catalytic Activity for Fuel Cells. Chemistry of Materials, 2010, 22, 3451-3456.	3.2	28

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127	Ethanol-Promoted High-Yield Growth of Few-Walled Carbon Nanotubes. Journal of Physical Chemistry C, 2010, 114, 6389-6395.	1.5	56
128	Ptâ˘'Cd and Ptâ˘'Hg Phases As High Activity Catalysts for Methanol and Formic Acid Oxidation. Journal of Physical Chemistry C, 2010, 114, 12545-12553.	1.5	19
129	Phase Behavior of Pseudobinary Precious Metalâ˘'Carbide Systems. Journal of Physical Chemistry C, 2010, 114, 21664-21671.	1.5	5
130	High Throughput X-ray Diffraction Analysis of Combinatorial Polycrystalline Thin Film Libraries. Analytical Chemistry, 2010, 82, 4564-4569.	3.2	5
131	High-Throughput Evaluation of Dealloyed Ptâ€"Zn Composition-Spread Thin Film for Methanol-Oxidation Catalysis. Journal of the Electrochemical Society, 2009, 156, B160.	1.3	37
132	Structural, electronic and optical properties of (Sc,Y)N solid solutions. Thin Solid Films, 2009, 517, 1607-1609.	0.8	28
133	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.	0.6	39
134	A model for calculating resputter rates in codeposition. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2008, 26, 1030-1036.	0.9	6
135	High mobility single crystalline ScN and single-orientation epitaxial YN on sapphire via magnetron sputtering. Journal of Applied Physics, 2008, 104, .	1.1	37
136	Getter sputtering system for high-throughput fabrication of composition spreads. Review of Scientific Instruments, 2007, 78, 072212.	0.6	31
137	Resputtering phenomena and determination of composition in codeposited films. Physical Review B, 2007, 76, .	1.1	16
138	An upgraded high-velocity dust particle accelerator at Concordia College in Moorhead, Minnesota. International Journal of Impact Engineering, 2006, 33, 402-409.	2.4	5
139	General counting formulae for factorized time correlation diagram analysis. Physica A: Statistical Mechanics and Its Applications, 2003, 320, 1-10.	1.2	5