Donald J Siegel

List of Publications by Year
in descending order

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126	9,968	31976	34986
papers	citations	53 h-index	98 g-index

134	134	134	10332
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	High capacity hydrogenstorage materials: attributes for automotive applications and techniques for materials discovery. Chemical Society Reviews, 2010, 39, 656-675.	38.1	1,008
2	Surface Chemistry Mechanism of Ultra-Low Interfacial Resistance in the Solid-State Electrolyte Li₇La₃Zr₂O₁₂. Chemistry of Materials, 2017, 29, 7961-7968.	6.7	612
3	Elastic Properties of the Solid Electrolyte Li₇La₃Zr₂O₁₂(LLZO). Chemistry of Materials, 2016, 28, 197-206.	6.7	445
4	Lithium Peroxide Surfaces Are Metallic, While Lithium Oxide Surfaces Are Not. Journal of the American Chemical Society, 2012, 134, 1093-1103.	13.7	331
5	Impact of air exposure and surface chemistry on Liâ€“Li₇La₃Zr₂O₁₂ interfacial resistance. Journal of Materials Chemistry A, 2017, 5, 13475-13487.	10.3	300
6	Charge transport in lithium peroxide: relevance for rechargeable metalâ€“air batteries. Energy and Environmental Science, 2013, 6, 2370.	30.8	293
7	Exceptional hydrogen storage achieved by screening nearly half a million metal-organic frameworks. Nature Communications, 2019, 10, 1568.	12.8	278
8	Electrochemical Window of the Li-Ion Solid Electrolyte Li₇La₃Zr₂O₁₂. ACS Energy Letters, 2017, 2, 462-468.	17.4	255
9	Adhesion, stability, and bonding at metal/metal-carbide interfaces: Al/WC. Surface Science, 2002, 498, 321-336.	1.9	224
10	Energy storage emerging: A perspective from the Joint Center for Energy Storage Research. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 12550-12557.	7.1	218
11	Adhesion, atomic structure, and bonding at theAl(111)/Î±â^'Al2O3(0001)interface: A first principles study. Physical Review B, 2002, 65, .	3.2	212
12	Theoretical Limits of Hydrogen Storage in Metalâ€“Organic Frameworks: Opportunities and Trade-Offs. Chemistry of Materials, 2013, 25, 3373-3382.	6.7	211
13	Precipitates in Alâ€“Cu alloys revisited: Atom-probe tomographic experiments and first-principles calculations of compositional evolution and interfacial segregation. Acta Materialia, 2011, 59, 6187-6204.	7.9	206
14	Enhanced Charge Transport in Amorphous Li₂O₂. Chemistry of Materials, 2014, 26, 2952-2959.	6.7	202
15	Grain Boundary Contributions to Li-Ion Transport in the Solid Electrolyte Li₇La₃Zr₂O₁₂ (LLZO). Chemistry of Materials, 2017, 29, 9639-9647.	6.7	189
16	Generalized stacking fault energies, ductilities, and twinnabilities of Ni and selected Ni alloys. Applied Physics Letters, 2005, 87, 121901.	3.3	167
17	An assessment of strategies for the development of solid-state adsorbents for vehicular hydrogen storage. Energy and Environmental Science, 2018, 11, 2784-2812.	30.8	162
18	Mechanical behavior of Li-ion-conducting crystalline oxide-based solid electrolytes: a brief review. Ionics, 2018, 24, 1271-1276.	2.4	136

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19	Grain Boundary Softening: A Potential Mechanism for Lithium Metal Penetration through Stiff Solid Electrolytes. ACS Applied Materials & Interfaces, 2018, 10, 38151-38158.	8.0	132
20	MOF-5 composites exhibiting improved thermal conductivity. International Journal of Hydrogen Energy, 2012, 37, 6109-6117.	7.1	130
21	First-principles study of metalâ€“carbide/nitride adhesion: Al/VC vs. Al/VN. Acta Materialia, 2002, 50, 619-631.	7.9	127
22	Ab initiostudy of Al-ceramic interfacial adhesion. Physical Review B, 2003, 67, .	3.2	127
23	Thermodynamic guidelines for the prediction of hydrogen storage reactions and their application to destabilized hydride mixtures. Physical Review B, 2007, 76, .	3.2	127
24	Increased volumetric hydrogen uptake of MOF-5 by powder densification. International Journal of Hydrogen Energy, 2012, 37, 2723-2727.	7.1	127
25	Balancing gravimetric and volumetric hydrogen density in MOFs. Energy and Environmental Science, 2017, 10, 2459-2471.	30.8	127
26	A Selfâ€Catalyzing Hydrogenâ€Storage Material. Angewandte Chemie - International Edition, 2008, 47, 882-887.	13.8	120
27	Improved Hydrogen Storage and Thermal Conductivity in High-Density MOF-5 Composites. Journal of Physical Chemistry C, 2012, 116, 20199-20212.	3.1	117
28	Low-temperature paddlewheel effect in glassy solid electrolytes. Nature Communications, 2020, 11, 1483.	12.8	102
29	Tuning the Adsorption of Polysulfides in Lithiumâ€“Sulfur Batteries with Metalâ€“Organic Frameworks. Chemistry of Materials, 2017, 29, 4932-4939.	6.7	98
30	Electrochemistry of Magnesium Electrolytes in Ionic Liquids for Secondary Batteries. ACS Applied Materials & Interfaces, 2014, 6, 18033-18039.	8.0	96
31	Optimizing Hydrogen Storage in MOFs through Engineering of Crystal Morphology and Control of Crystal Size. Journal of the American Chemical Society, 2021, 143, 10727-10734.	13.7	95
32	Embedded-atom-method tantalum potential developed by the force-matching method. Physical Review B, 2003, 67, .	3.2	93
33	Kinetic Stability of MOF-5 in Humid Environments: Impact of Powder Densification, Humidity Level, and Exposure Time. Langmuir, 2015, 31, 4988-4995.	3.5	88
34	Compositional evolution of Q-phase precipitates in an aluminum alloy. Acta Materialia, 2014, 75, 322-336.	7.9	83
35	Electronic structure of Li2O2 {0001} surfaces. Journal of Materials Science, 2012, 47, 7564-7570.	3.7	82
36	Simultaneous Segregation at Coherent and Semicoherent Heterophase Interfaces. Physical Review Letters, 2010, 105, 076102.	7.8	80

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37	How Dopants Can Enhance Charge Transport in Li₂O₂. Chemistry of Materials, 2015, 27, 839-847.	6.7	79
38	Development of glue-type potentials for the Alâ€“Pb system: phase diagram calculation. Acta Materialia, 2000, 48, 1753-1761.	7.9	77
39	Discovery of novel hydrogen storage materials: an atomic scale computational approach. Journal of Physics Condensed Matter, 2008, 20, 064228.	1.8	75
40	Intrinsic Conductivity in Sodiumâ€“Air Battery Discharge Phases: Sodium Superoxide vs Sodium Peroxide. Chemistry of Materials, 2015, 27, 3852-3860.	6.7	73
41	Comparing van der Waals Density Functionals for CO₂ Adsorption in Metal Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 16957-16968.	3.1	72
42	First-principles study of the solubility, diffusion, and clustering of C in Ni. Physical Review B, 2003, 68, .	3.2	71
43	Reaction energetics and crystal structure ofLi4BN3H10from first principles. Physical Review B, 2007, 75, .	3.2	70
44	Correlating lattice distortions, ion migration barriers, and stability in solid electrolytes. Journal of Materials Chemistry A, 2019, 7, 3216-3227.	10.3	68
45	Thermophysical properties of MOF-5 powders. Microporous and Mesoporous Materials, 2014, 185, 235-244.	4.4	67
46	Correlating Li/O₂ Cell Capacity and Product Morphology with Discharge Current. ACS Applied Materials & Interfaces, 2015, 7, 7670-7678.	8.0	66
47	First-Principles Study of Redox End Members in Lithiumâ€“Sulfur Batteries. Journal of Physical Chemistry C, 2015, 119, 4675-4683.	3.1	65
48	Crystal Surface and State of Charge Dependencies of Electrolyte Decomposition on LiMn₂O₄Cathode. Journal of the Electrochemical Society, 2014, 161, E3059-E3065.	2.9	63
49	Thermodynamic screening of metal-substituted MOFs for carbon capture. Physical Chemistry Chemical Physics, 2013, 15, 4573.	2.8	62
50	Predicting Methane Storage in Open-Metal-Site Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2015, 119, 13451-13458.	3.1	62
51	Water Adsorption and Insertion in MOF-5. ACS Omega, 2017, 2, 4921-4928.	3.5	59
52	Identifying the Discharge Product and Reaction Pathway for a Secondary Mg/O₂ Battery. Chemistry of Materials, 2015, 27, 7564-7568.	6.7	57
53	Correlating Macro and Atomic Structure with Elastic Properties and Ionic Transport of Glassy Li₂Sâ€P₂S₅ (LPS) Solid Electrolyte for Solidâ€State Li Metal Batteries. Advanced Energy Materials, 2020, 10, 2000335.	19.5	56
54	Impact of Space-Charge Layers on Sudden Death in Li/O₂ Batteries. Journal of Physical Chemistry Letters, 2015, 6, 3017-3022.	4.6	53

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55	Estimation of system-level hydrogen storage for metal-organic frameworks with high volumetric storage density. International Journal of Hydrogen Energy, 2019, 44, 15135-15145.	7.1	53
56	Dynamics of Hydroxyl Anions Promotes Lithium Ion Conduction in Antiperovskite Li₂OHCl. Chemistry of Materials, 2020, 32, 8481-8491.	6.7	53
57	Predicting hydrogen storage in MOFs via machine learning. Patterns, 2021, 2, 100291.	5.9	51
58	Investigation of vinyl phosphonic acid/hydroxylated Î±-Al2O3() reaction enthalpies. Surface Science, 2001, 494, 1-20.	1.9	48
59	Atomic layer deposition and first principles modeling of glassy Li₃BO₃â€“Li₂CO₃ electrolytes for solid-state Li metal batteries. Journal of Materials Chemistry A, 2018, 6, 19425-19437.	10.3	48
60	Elucidating the mobility of H⁺and Li⁺ions in (Li_{6.25â^'x}H_xAl_{0.25})La₃Zr₂O₁₂viacorrelative neutron and electron spectroscopy. Energy and Environmental Science, 2019, 12, 945-951.	33.8	48
61	Adhesion, lubrication and wear on the atomic scale. Surface and Interface Analysis, 2001, 31, 619-626.	1.8	46
62	Intrinsic Conductivity in Magnesiumâ€“Oxygen Battery Discharge Products: MgO and MgO₂. Chemistry of Materials, 2017, 29, 3152-3163.	6.7	46
63	Computational Screening of Hydration Reactions for Thermal Energy Storage: New Materials and Design Rules. Chemistry of Materials, 2018, 30, 2006-2017.	6.7	45
64	Hydrogen storage properties of 2LiNH2+LiBH4+MgH2. Journal of Alloys and Compounds, 2007, 446-447, 345-349.	5.5	44
65	Thermodynamic Overpotentials and Nucleation Rates for Electrodeposition on Metal Anodes. ACS Applied Materials & Interfaces, 2019, 11, 7954-7964.	8.0	44
66	Methane Storage in Metal-Substituted Metalâ€“Organic Frameworks: Thermodynamics, Usable Capacity, and the Impact of Enhanced Binding Sites. Journal of Physical Chemistry C, 2014, 118, 2929-2942.	3.1	43
67	High throughput screening of the ternary LiNH2â€“MgH2â€“LiBH4 phase diagram. Journal of Alloys and Compounds, 2007, 446-447, 355-359.	5.5	42
68	Theoretical Limiting Potentials in Mg/O₂ Batteries. Chemistry of Materials, 2016, 28, 1390-1401.	6.7	42
69	Interface-Induced Renormalization of Electrolyte Energy Levels in Magnesium Batteries. Journal of Physical Chemistry Letters, 2016, 7, 874-881.	4.6	39
70	Computational study of carbon segregation and diffusion within a nickel grain boundary. Acta Materialia, 2005, 53, 87-96.	7.9	36
71	Surface-Mediated Solvent Decomposition in Liâ€“Air Batteries: Impact of Peroxide and Superoxide Surface Terminations. Journal of Physical Chemistry C, 2015, 119, 9050-9060.	3.1	36
72	Why Do Grain Boundaries Exhibit Finite Facet Lengths?. Physical Review Letters, 2003, 90, 246102.	7.8	34

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73	Ion Pairing and Diffusion in Magnesium Electrolytes Based on Magnesium Borohydride. ACS Applied Materials & Interfaces, 2017, 9, 43755-43766.	8.0	34
74	Hydrogen permeation and diffusion in densified MOF-5 pellets. International Journal of Hydrogen Energy, 2013, 38, 3268-3274.	7.1	30
75	Thermophysical properties of LiFePO4 cathodes with carbonized pitch coatings and organic binders: Experiments and first-principles modeling. Journal of Power Sources, 2014, 251, 8-13.	7.8	30
76	Adiabatic and Nonadiabatic Charge Transport in Liâ€“S Batteries. Chemistry of Materials, 2018, 30, 915-928.	6.7	30
77	Lithiumâ€“oxygen batteries: At a crossroads?. Current Opinion in Electrochemistry, 2017, 6, 100-107.	4.8	28
78	Reaction Pathways for Solvent Decomposition on Magnesium Anodes. Journal of Physical Chemistry C, 2018, 122, 10714-10724.	3.1	28
79	Establishing a unified framework for ion solvation and transport in liquid and solid electrolytes. Trends in Chemistry, 2021, 3, 807-818.	8.5	27
80	Anisotropic thermal transport in MOF-5 composites. International Journal of Heat and Mass Transfer, 2015, 82, 250-258.	4.8	26
81	Mg/O₂ Battery Based on the Magnesiumâ€“Aluminum Chloride Complex (MACC) Electrolyte. Chemistry of Materials, 2016, 28, 7629-7637.	6.7	25
82	Modeling the Interface between Lithium Metal and Its Native Oxide. ACS Applied Materials & Interfaces, 2020, 12, 46015-46026.	8.0	25
83	Predicting Charge Transfer Stability between Sulfide Solid Electrolytes and Li Metal Anodes. ACS Energy Letters, 2021, 6, 150-157.	17.4	24
84	Predicting Wettability and the Electrochemical Window of Lithium-Metal/Solid Electrolyte Interfaces. ACS Applied Materials & Interfaces, 2019, 11, 39940-39950.	8.0	22
85	Computational Model of Magnesium Deposition and Dissolution for Property Determination via Cyclic Voltammetry. Journal of the Electrochemical Society, 2016, 163, A1813-A1821.	2.9	21
86	Thermodynamic Assessment of Coating Materials for Solid-State Li, Na, and K Batteries. ACS Applied Materials & Interfaces, 2019, 11, 36607-36615.	8.0	21
87	Impact of Stoichiometry on the Hydrogen Storage Properties of LiNH₂â^'LiBH₄â^'MgH₂ Ternary Composites. Journal of Physical Chemistry C, 2009, 113, 2004-2013.	3.1	20
88	Charge Transport in Alkali-Metal Superoxides: A Systematic First-Principles Study. Chemistry of Materials, 2019, 31, 9156-9167.	6.7	19
89	Sustainable Mobility, Future Fuels, and the Periodic Table. Journal of Chemical Education, 2013, 90, 440-445.	2.3	17
90	Synthesis of Antiperovskite Solid Electrolytes: Comparing Li₃SI, Na₃SI, and Ag₃SI. Inorganic Chemistry, 2020, 59, 11244-11247.	4.0	16

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91	Stability of MOF-5 in a hydrogen gas environment containing fueling station impurities. International Journal of Hydrogen Energy, 2016, 41, 9374-9382.	7.1	15
92	Understanding the Magnetocatalytic Effect: Magnetism as a Driving Force for Surface Segregation. Physical Review Letters, 2004, 92, 086101.	7.8	13
93	Exploring the Synthesis of Alkali Metal Anti-perovskites. Chemistry of Materials, 2022, 34, 947-958.	6.7	13
94	Computational Identification and Experimental Demonstration of Highâ€Performance Methane Sorbents. Angewandte Chemie - International Edition, 2022, 61, e202203575.	13.8	13
95	Non-aqueous Metalâ€“Oxygen Batteries: Past, Present, and Future. Green Energy and Technology, 2015, , 511-539.	0.6	11
96	Multivalent Ion Transport in Anti-Perovskite Solid Electrolytes. Chemistry of Materials, 2021, 33, 2187-2197.	6.7	9
97	Education on vehicle electrification: Battery Systems, Fuel Cells, and Hydrogen. , 2010, , .		8
98	Anisotropic Elastic Properties of Battery Anodes. Journal of the Electrochemical Society, 2020, 167, 110550.	2.9	8
99	Gas Evolution in Li-Ion Batteries: Modeling Ethylene Carbonate Decomposition on LiCoO₂ in the Presence of Surface Magnetism. Journal of Physical Chemistry C, 2020, 124, 24097-24104.	3.1	6
100	NGenE 2021: Electrochemistry Is Everywhere. ACS Energy Letters, 2022, 7, 368-374.	17.4	6
101	Ion Migration Mechanisms in the Sodium Sulfide Solid Electrolyte Na_{3â€“x}Sb_{1â€“x}W_xS₄. Chemistry of Materials, 2022, 34, 4166-4171.	6.7	6
102	Electronic Structure and Bonding at the Al-terminated Al(111)/Î±-Al₂O₃(0001) Interface: A First Principles Study. Materials Research Society Symposia Proceedings, 2000, 654, 421.	0.1	5
103	Machine learning reveals factors that control ion mobility in anti-perovskite solid electrolytes. Journal of Materials Chemistry A, 2022, 10, 15169-15182.	10.3	5
104	Understanding the Structural Disorder Related to Ionic Conductivity Enhancement in Anti-Perovskite Ion Conductors. ECS Meeting Abstracts, 2020, MA2020-02, 967-967.	0.0	2
105	Computational Identification and Experimental Demonstration of Highâ€Performance Methane Sorbents. Angewandte Chemie, 2022, 134, .	2.0	2
106	Stoichiometry and Adhesion of Al/WC. Materials Research Society Symposia Proceedings, 2001, 677, 4251.	0.1	1
107	Solidâ€State Batteries: Correlating Macro and Atomic Structure with Elastic Properties and Ionic Transport of Glassy Li₂Sâ€P₂S₅ (LPS) Solid Electrolyte for Solidâ€State Li Metal Batteries (Adv. Energy Mater. 19/2020). Advanced Energy Materials, 2020, 10, 2070085.	19.5	1
108	Predicting Hydrogen Storage in Mofs <i>via</i> Machine Learning. SSRN Electronic Journal, 0, , .	0.4	1

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109	(Invited) Stability and Kinetics of the Li/Solid-State Electrolyte Interface. ECS Meeting Abstracts, 2018, , .	0.0	0
110	(Invited) Tuning Ion Mobility in Solid Electrolytes Via Lattice Disorder. ECS Meeting Abstracts, 2018, , .	0.0	0
111	Adiabatic and Nonadiabatic Charge Transport in Li-S Batteries. ECS Meeting Abstracts, 2018, , .	0.0	0
112	(Invited) Atomic Scale Simulations of Interfacial Phenomena in Solid Electrolytes. ECS Meeting Abstracts, 2018, , .	0.0	0
113	Grain Boundary Contributions to Li-Ion Transport in the Solid Electrolyte Li7La3Zr2O12. ECS Meeting Abstracts, 2018, , .	0.0	0
114	Tuning the Adsorption of Polysulfides(Li2Sx) in Lithium-Sulfur Batteries with Metal-Organic Frameworks(MOFs). ECS Meeting Abstracts, 2018, , .	0.0	0
115	First-Principles Models of Phenomena at Li-Metal/Anti-Perovskite Li3ocl Solid Electrolyte Interfaces. ECS Meeting Abstracts, 2018, , .	0.0	0
116	Atomic Layer Deposition of Ultrathin Lithium Borate Solid Electrolytes. ECS Meeting Abstracts, 2018, , .	0.0	0
117	Maximizing Ionic Mobility By Lattice Disorder in Anti-Perovskite Solid Electrolytes. ECS Meeting Abstracts, 2018, , .	0.0	0
118	Surface Chemistry Mechanism of Ultra-Low Interfacial Resistance in the Solid-State Electrolyte Li7La3Zr2O12. ECS Meeting Abstracts, 2018, , .	0.0	0
119	(Invited) Cooperative Ion Migration in Li-Ion Conducting Glasses. ECS Meeting Abstracts, 2019, , .	0.0	0
120	(Invited) Complex Ion Migration Mechanisms in Glassy Lithium Solid Electrolytes. ECS Meeting Abstracts, 2019, , .	0.0	0
121	Atomic-Scale Simulations of Grain Boundary Mechanical Properties in the Solid Electrolyte Li7La3Zr2O12. ECS Meeting Abstracts, 2019, , .	0.0	0
122	Atomic Layer Deposition of Ultrathin Glassy Lithium Borate-Carbonate Solid Electrolytes. ECS Meeting Abstracts, 2019, , .	0.0	0
123	(Invited) Computational Discovery of Metal-Organic Frameworks for Hydrogen Storage: Combining High-Throughput Screening, Machine Learning, and Experimental Demonstration. ECS Meeting Abstracts, 2019, , .	0.0	0
124	Potential Solid Electrolytes for Multivalent-Ions Based on the Anti-Perovskite Structure. ECS Meeting Abstracts, 2020, MA2020-01, 575-575.	0.0	0
125	Tuning Ionic Conductivity in Sodium Anti-Perovskite Ionic Conductors. ECS Meeting Abstracts, 2020, MA2020-02, 945-945.	0.0	0
126	Temperature-Dependent Atomistic Dynamics Correlated to Cation Transport in Cluster-Ion Anti-Perovskites. ECS Meeting Abstracts, 2020, MA2020-02, 966-966.	0.0	0