

# Jeffrey C Grossman

## List of Publications by Year in descending order

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127  
papers

8,310  
citations

50273

46  
h-index

48312

88  
g-index

129  
all docs

129  
docs citations

129  
times ranked

12707  
citing authors

#	ARTICLE	IF	CITATIONS
1	Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties. <i>Physical Review Letters</i> , 2018, 120, 145301.	7.8	1,102
2	Exciton Radiative Lifetimes in Two-Dimensional Transition Metal Dichalcogenides. <i>Nano Letters</i> , 2015, 15, 2794-2800.	9.1	517
3	Multilayer Nanoporous Graphene Membranes for Water Desalination. <i>Nano Letters</i> , 2016, 16, 1027-1033.	9.1	331
4	Scalable enhancement of graphene oxide properties by thermally driven phase transformation. <i>Nature Chemistry</i> , 2014, 6, 151-158.	13.6	326
5	Quantifying the potential of ultra-permeable membranes for water desalination. <i>Energy and Environmental Science</i> , 2014, 7, 1134-1141.	30.8	282
6	Templated assembly of photoswitches significantly increases the energy-storage capacity of solar thermal fuels. <i>Nature Chemistry</i> , 2014, 6, 441-447.	13.6	261
7	Ultralow thermal conductivity in all-inorganic halide perovskites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 8693-8697.	7.1	246
8	Atomistic understandings of reduced graphene oxide as an ultrathin-film nanoporous membrane for separations. <i>Nature Communications</i> , 2015, 6, 8335.	12.8	214
9	Optically-controlled long-term storage and release of thermal energy in phase-change materials. <i>Nature Communications</i> , 2017, 8, 1446.	12.8	210
10	Polarity governs atomic interaction through two-dimensional materials. <i>Nature Materials</i> , 2018, 17, 999-1004.	27.5	182
11	Water permeability of nanoporous graphene at realistic pressures for reverse osmosis desalination. <i>Journal of Chemical Physics</i> , 2014, 141, 074704.	3.0	163
12	Self-Driven Photodetector and Ambipolar Transistor in Atomically Thin GaTe-MoS <sub>2</sub> vdW Heterostructure. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 2533-2539.	8.0	160
13	Machine Learning Enabled Computational Screening of Inorganic Solid Electrolytes for Suppression of Dendrite Formation in Lithium Metal Anodes. <i>ACS Central Science</i> , 2018, 4, 996-1006.	11.3	158
14	Optical and Electronic Properties of Two-Dimensional Layered Materials. <i>Nanophotonics</i> , 2017, 6, 479-493.	6.0	145
15	Sleep quality, duration, and consistency are associated with better academic performance in college students. <i>Npj Science of Learning</i> , 2019, 4, 16.	2.8	133
16	Atomic Structure and Dynamics of Single Platinum Atom Interactions with Monolayer MoS <sub>2</sub> . <i>ACS Nano</i> , 2017, 11, 3392-3403.	14.6	126
17	Correlations from Ion Pairing and the Nernst-Einstein Equation. <i>Physical Review Letters</i> , 2019, 122, 136001.	7.8	101
18	Ionic Highways from Covalent Assembly in Highly Conducting and Stable Anion Exchange Membrane Fuel Cells. <i>Journal of the American Chemical Society</i> , 2019, 141, 18152-18159.	13.7	99

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19	Molecularly Engineered Azobenzene Derivatives for High Energy Density Solid-State Solar Thermal Fuels. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 8679-8687.	8.0	97
20	Solid-State Solar Thermal Fuels for Heat Release Applications. <i>Advanced Energy Materials</i> , 2016, 6, 1502006.	19.5	94
21	Laser-sculptured ultrathin transition metal carbide layers for energy storage and energy harvesting applications. <i>Nature Communications</i> , 2019, 10, 3112.	12.8	91
22	Photon energy storage materials with high energy densities based on diacetylene-azobenzene derivatives. <i>Journal of Materials Chemistry A</i> , 2016, 4, 16157-16165.	10.3	86
23	Graph dynamical networks for unsupervised learning of atomic scale dynamics in materials. <i>Nature Communications</i> , 2019, 10, 2667.	12.8	82
24	Identifying and Eliminating Emissive Sub-bandgap States in Thin Films of PbS Nanocrystals. <i>Advanced Materials</i> , 2015, 27, 4481-4486.	21.0	77
25	Insight on Tricalcium Silicate Hydration and Dissolution Mechanism from Molecular Simulations. <i>ACS Applied Materials &amp; Interfaces</i> , 2015, 7, 14726-14733.	8.0	76
26	Photovoltaic Performance of PbS Quantum Dots Treated with Metal Salts. <i>ACS Nano</i> , 2016, 10, 3382-3388.	14.6	75
27	Photoswitchable Molecular Rings for Solar-Thermal Energy Storage. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 854-860.	4.6	74
28	Failing Forward: Stability of Transparent Electrodes Based on Metal Nanowire Networks. <i>Advanced Materials</i> , 2021, 33, e2004356.	21.0	74
29	Solar energy generation in three dimensions. <i>Energy and Environmental Science</i> , 2012, 5, 6880.	30.8	73
30	Atomically Flat Zigzag Edges in Monolayer MoS <sub>2</sub> by Thermal Annealing. <i>Nano Letters</i> , 2017, 17, 5502-5507.	9.1	70
31	Role of Structural Defects in the Water Adsorption Properties of MOF-801. <i>Journal of Physical Chemistry C</i> , 2018, 122, 5545-5552.	3.1	68
32	High-Efficiency Thermoelectrics with Functionalized Graphene. <i>Nano Letters</i> , 2015, 15, 2830-2835.	9.1	67
33	Kinetics of Sorption in Hygroscopic Hydrogels. <i>Nano Letters</i> , 2022, 22, 1100-1107.	9.1	65
34	Toward Designing Highly Conductive Polymer Electrolytes by Machine Learning Assisted Coarse-Grained Molecular Dynamics. <i>Chemistry of Materials</i> , 2020, 32, 4144-4151.	6.7	63
35	Double-Sided Graphene Oxide Encapsulated Silver Nanowire Transparent Electrode with Improved Chemical and Electrical Stability. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 17909-17920.	8.0	60
36	The Characterization, Stability, and Reactivity of Synthetic Calcium Silicate Surfaces from First Principles. <i>Journal of Physical Chemistry C</i> , 2014, 118, 15214-15219.	3.1	58

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37	Optically-regulated thermal energy storage in diverse organic phase-change materials. <i>Chemical Communications</i> , 2018, 54, 10722-10725.	4.1	55
38	MoS <sub>2</sub> Enhanced T-Phase Stabilization and Tunability Through Alloying. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2304-2309.	4.6	54
39	Ultralong 1D Vacancy Channels for Rapid Atomic Migration during 2D Void Formation in Monolayer MoS <sub>2</sub> . <i>ACS Nano</i> , 2018, 12, 7721-7730.	14.6	54
40	Thermodynamic-driven polychromatic quantum dot patterning for light-emitting diodes beyond eye-limiting resolution. <i>Nature Communications</i> , 2020, 11, 3040.	12.8	53
41	High Surface Reactivity and Water Adsorption on NiFe <sub>2</sub> O <sub>4</sub> (111) Surfaces. <i>Journal of Physical Chemistry C</i> , 2013, 117, 5678-5683.	3.1	52
42	Enhanced Cell Capture on Functionalized Graphene Oxide Nanosheets through Oxygen Clustering. <i>ACS Nano</i> , 2017, 11, 1548-1558.	14.6	52
43	Hierarchical visualization of materials space with graph convolutional neural networks. <i>Journal of Chemical Physics</i> , 2018, 149, 174111.	3.0	52
44	Capillary-fed, thin film evaporation devices. <i>Journal of Applied Physics</i> , 2020, 128, .	2.5	51
45	Charting lattice thermal conductivity for inorganic crystals and discovering rare earth chalcogenides for thermoelectrics. <i>Energy and Environmental Science</i> , 2021, 14, 3559-3566.	30.8	51
46	Origins of the Stokes Shift in PbS Quantum Dots: Impact of Polydispersity, Ligands, and Defects. <i>ACS Nano</i> , 2018, 12, 2838-2845.	14.6	50
47	Unveiling the phonon scattering mechanisms in half-Heusler thermoelectric compounds. <i>Energy and Environmental Science</i> , 2020, 13, 5165-5176.	30.8	49
48	Interplay between intrinsic defects, doping, and free carrier concentration in SrTiO <sub>3</sub> thin films. <i>Physical Review B</i> , 2012, 85, .	3.2	46
49	Strain-induced accelerated asymmetric spatial degradation of polymeric vascular scaffolds. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 2640-2645.	7.1	46
50	Role of solvent-anion charge transfer in oxidative degradation of battery electrolytes. <i>Nature Communications</i> , 2019, 10, 3360.	12.8	46
51	Inorganic Cage Motion Dominates Excited-State Dynamics in 2D-Layered Perovskites (C <sub>x</sub> H <sub>2x+1</sub> NH <sub>3</sub> ) <sub>2</sub> PbI <sub>4</sub> (C <sub>x</sub> = 4-9). <i>Journal of Physical Chemistry C</i> , 2019, 123, 27904-27916.		
52	Revealing the Cluster-Cloud and Its Role in Nanocrystallization. <i>Advanced Materials</i> , 2019, 31, e1808225.	21.0	41
53	Electron-hole separation in ferroelectric oxides for efficient photovoltaic responses. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 6566-6571.	7.1	40
54	Rethinking Coal: Thin Films of Solution Processed Natural Carbon Nanoparticles for Electronic Devices. <i>Nano Letters</i> , 2016, 16, 2951-2957.	9.1	39

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55	Preserving nanoscale features in polymers during laser induced graphene formation using sequential infiltration synthesis. <i>Nature Communications</i> , 2020, 11, 3636.	12.8	39
56	Charge separation in nanoscale photovoltaic materials: recent insights from first-principles electronic structure theory. <i>Journal of Materials Chemistry</i> , 2010, 20, 1053-1061.	6.7	38
57	Room Temperature Multiferroicity of Charge Transfer Crystals. <i>ACS Nano</i> , 2015, 9, 9373-9379.	14.6	38
58	Heat Conduction in Nanostructured Materials Predicted by Phonon Bulk Mean Free Path Distribution. <i>Journal of Heat Transfer</i> , 2015, 137, .	2.1	36
59	Photoluminescent Arrays of Nanopatterned Monolayer MoS <sub>2</sub> . <i>Advanced Functional Materials</i> , 2017, 27, 1703688.	14.9	35
60	Fundamental Insights on Hydration Environment of Boric Acid and Its Role in Separation from Saline Water. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1438-1445.	3.1	35
61	Conformal Electroplating of Azobenzene-Based Solar Thermal Fuels onto Large-Area and Fiber Geometries. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 26319-26325.	8.0	33
62	Laser-Induced Graphene from Polyimide and Polyethersulfone Precursors as a Sensing Electrode in Anodic Stripping Voltammetry. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 48511-48517.	8.0	33
63	Mesoscale modeling of phononic thermal conductivity of porous Si: interplay between porosity, morphology and surface roughness. <i>Journal of Computational Electronics</i> , 2012, 11, 8-13.	2.5	32
64	Atomic Structure and Dynamics of Defects in 2D MoS <sub>2</sub> Bilayers. <i>ACS Omega</i> , 2017, 2, 3315-3324.	3.5	32
65	Origins of hole traps in hydrogenated nanocrystalline and amorphous silicon revealed through machine learning. <i>Physical Review B</i> , 2014, 89, .	3.2	31
66	Striated 2D Lattice with Sub- $\mu\text{m}$ 1D Etch Channels by Controlled Thermally Induced Phase Transformations of PdSe <sub>2</sub> . <i>Advanced Materials</i> , 2019, 31, e1904251.	21.0	31
67	Predicting charge density distribution of materials using a local-environment-based graph convolutional network. <i>Physical Review B</i> , 2019, 100, .	3.2	31
68	Atomic structure and defect dynamics of monolayer lead iodide nanodisks with epitaxial alignment on graphene. <i>Nature Communications</i> , 2020, 11, 823.	12.8	31
69	Silver Nanowire Back Electrode Stabilized with Graphene Oxide Encapsulation for Inverted Semitransparent Organic Solar Cells with Longer Lifetime. <i>ACS Applied Energy Materials</i> , 2021, 4, 1431-1441.	5.1	31
70	Mpemba-Like Behavior in Carbon Nanotube Resonators. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2011, 42, 3907-3912.	2.2	30
71	Stress effects on the Raman spectrum of an amorphous material: Theory and experiment on $\alpha$ -Si:H. <i>Physical Review B</i> , 2015, 92, .	3.2	30
72	Torsional Deformations in Subnanometer MoS Interconnecting Wires. <i>Nano Letters</i> , 2016, 16, 1210-1217.	9.1	30

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73	Atomic Structure and Dynamics of Self-Limiting Sub-Nanometer Pores in Monolayer WS <sub>2</sub> . ACS Nano, 2018, 12, 11638-11647.	14.6	30
74	Solvent- and Anion-Dependent Li <sup>+</sup> O <sub>2</sub> <sup>-</sup> Coupling Strength and Implications on the Thermodynamics and Kinetics of LiO <sub>2</sub> Batteries. Journal of Physical Chemistry C, 2020, 124, 4953-4967.	3.1	29
75	Three-dimensional photovoltaics. Applied Physics Letters, 2010, 96, 071902.	3.3	28
76	Band Engineering by Controlling vdW Epitaxy Growth Mode in 2D Gallium Chalcogenides. Advanced Materials, 2016, 28, 7375-7382.	21.0	28
77	Conductive carbonaceous membranes: recent progress and future opportunities. Journal of Materials Chemistry A, 2021, 9, 3270-3289.	10.3	28
78	Computer calculations across time and length scales in photovoltaic solar cells. Energy and Environmental Science, 2016, 9, 2197-2218.	30.8	27
79	Effect of Chemical Variations in the Structure of Poly(ethylene oxide)-Based Polymers on Lithium Transport in Concentrated Electrolytes. Chemistry of Materials, 2020, 32, 121-126.	6.7	27
80	Low-frequency Raman spectrum of 2D layered perovskites: Local atomistic motion or superlattice modes?. Journal of Chemical Physics, 2020, 153, 044710.	3.0	26
81	Highly Conductive and Permeable Nanocomposite Ultrafiltration Membranes Using Laser-Reduced Graphene Oxide. Nano Letters, 2021, 21, 2429-2435.	9.1	26
82	A 3D-printed molecular ferroelectric metamaterial. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 27204-27210.	7.1	25
83	Upgrading carbonaceous materials: Coal, tar, pitch, and beyond. Matter, 2022, 5, 430-447.	10.0	24
84	Epitaxial Templating of Two-Dimensional Metal Chloride Nanocrystals on Monolayer Molybdenum Disulfide. ACS Nano, 2017, 11, 6404-6415.	14.6	20
85	Investigation of a Quantum Monte Carlo Protocol To Achieve High Accuracy and High-Throughput Materials Formation Energies. Journal of Chemical Theory and Computation, 2017, 13, 1943-1951.	5.3	20
86	Blue Light Emitting Defective Nanocrystals Composed of Earth-Abundant Elements. Angewandte Chemie - International Edition, 2020, 59, 860-867.	13.8	20
87	All-polymeric control of nanoferronics. Science Advances, 2015, 1, e1501264.	10.3	18
88	Catalyst Self-Assembly for Scalable Patterning of Sub 10 nm Ultrahigh Aspect Ratio Nanopores in Silicon. ACS Applied Materials & Interfaces, 2016, 8, 8043-8049.	8.0	18
89	High-Pressure-Sintering-Induced Microstructural Engineering for an Ultimate Phonon Scattering of Thermoelectric Half-Heusler Compounds. Small, 2021, 17, e2102045.	10.0	17
90	Charge Density and Redox Potential of LiNiO <sub>2</sub> Using Ab Initio Diffusion Quantum Monte Carlo. Journal of Physical Chemistry C, 2020, 124, 5893-5901.	3.1	16

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91	Transport-Based Modeling of Bubble Nucleation on Gas Evolving Electrodes. <i>Langmuir</i> , 2020, 36, 15112-15118.	3.5	15
92	Quantitative Mapping of Molecular Substituents to Macroscopic Properties Enables Predictive Design of Oligoethylene Glycol-Based Lithium Electrolytes. <i>ACS Central Science</i> , 2020, 6, 1115-1128.	11.3	15
93	Chemically Driven Interfacial Coupling in Charge-Transfer Mediated Functional Superstructures. <i>Nano Letters</i> , 2016, 16, 2851-2859.	9.1	14
94	Natural Carbon By-Products for Transparent Heaters: The Case of Steam-Cracker Tar. <i>Advanced Materials</i> , 2019, 31, e1900331.	21.0	13
95	2D Monolayers for Superior Transparent Electromagnetic Interference Shielding. <i>ACS Nano</i> , 2022, 16, 9498-9509.	14.6	13
96	Tuning the Potential Energy Landscape to Suppress Ostwald Ripening in Surface-Supported Catalyst Systems. <i>Nano Letters</i> , 2019, 19, 8388-8398.	9.1	12
97	Blue Light Emitting Defective Nanocrystals Composed of Earth-Abundant Elements. <i>Angewandte Chemie</i> , 2020, 132, 870-877.	2.0	12
98	Atomic Structure of Dislocations and Grain Boundaries in Two-Dimensional PtSe <sub>2</sub> . <i>ACS Nano</i> , 2021, 15, 16748-16759.	14.6	12
99	Screening and Understanding Li Adsorption on Two-Dimensional Metallic Materials by Learning Physics and Physics-Simplified Learning. <i>Jacs Au</i> , 2021, 1, 1904-1914.	7.9	12
100	Oxynitride-Encapsulated Silver Nanowire Transparent Electrode with Enhanced Thermal, Electrical, and Chemical Stability. <i>ACS Applied Materials &amp; Interfaces</i> , 2022, 14, 4423-4433.	8.0	12
101	Atoms to fibers: Identifying novel processing methods in the synthesis of pitch-based carbon fibers. <i>Science Advances</i> , 2022, 8, eabn1905.	10.3	12
102	Optimization of the Thermoelectric Figure of Merit in Crystalline C <sub>60</sub> with Intercalation Chemistry. <i>Nano Letters</i> , 2016, 16, 4203-4209.	9.1	10
103	Freestanding Organic Charge-Transfer Conformal Electronics. <i>Nano Letters</i> , 2018, 18, 4346-4354.	9.1	10
104	Bandlike Transport in PbS Quantum Dot Superlattices with Quantum Confinement. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3756-3762.	4.6	10
105	Engineering Efficient p-Type TMD/Metal Contacts Using Fluorographene as a Buffer Layer. <i>Advanced Electronic Materials</i> , 2017, 3, 1600318.	5.1	9
106	Importance of Equilibration Method and Sampling for <i>Ab Initio</i> Molecular Dynamics Simulations of Solvent-Lithium-Salt Systems in Lithium-Oxygen Batteries. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7255-7266.	5.3	9
107	Laser-Induced Tar-Mediated Sintering of Metals and Refractory Carbides in Air. <i>ACS Nano</i> , 2020, 14, 10413-10420.	14.6	9
108	Electronic, Structural, and Magnetic Upgrading of Coal-Based Products through Laser Annealing. <i>ACS Nano</i> , 2022, 16, 2101-2109.	14.6	9

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109	Ultra-high aspect ratio functional nanoporous silicon via nucleated catalysts. RSC Advances, 2017, 7, 11537-11542.	3.6	8
110	Functionalized Graphene Superlattice as a Single-Sheet Solar Cell. Advanced Functional Materials, 2015, 25, 5199-5205.	14.9	7
111	Novel nanomaterials for water desalination technology. , 2013, , .		6
112	Design Rules for Transparent Push-Pull Electron Acceptors: A Case Study on Perylene-dimide Derivatives. Journal of Physical Chemistry Letters, 2020, 11, 9265-9271.	4.6	6
113	Laser-Induced Cooperative Transition in Molecular Electronic Crystal. Advanced Materials, 2021, 33, e2103000.	21.0	6
114	Charge Transport in Highly Heterogeneous Natural Carbonaceous Materials. Advanced Functional Materials, 2019, 29, 1904283.	14.9	5
115	Emerging Magnetic Interactions in van der Waals Heterostructures. Nano Letters, 2020, 20, 7852-7859.	9.1	5
116	Emerged Metallicity in Molecular Ferromagnetic Wires. Nano Letters, 2021, 21, 9746-9753.	9.1	5
117	Numerical validation of the dusty-gas model for binary diffusion in low aspect ratio capillaries. Physics of Fluids, 2021, 33, .	4.0	4
118	Printing Air-Stable High-Tc Molecular Magnet with Tunable Magnetic Interaction. Nano Letters, 2022, 22, 545-553.	9.1	4
119	Nanostructured Bulk-Heterojunction Solar Cells Based on Amorphous Carbon. ACS Energy Letters, 2017, 2, 882-888.	17.4	3
120	Nanoporous Silicon-Assisted Patterning of Monolayer MoS <sub>2</sub> with Thermally Controlled Porosity: A Scalable Method for Diverse Applications. ACS Applied Nano Materials, 2018, 1, 3548-3556.	5.0	3
121	Cyclobutene based macrocycles. Materials Chemistry Frontiers, 2020, 4, 3529-3538.	5.9	3
122	Adsorption-based membranes for air separation using transition metal oxides. Nanoscale Advances, 2021, 3, 4502-4512.	4.6	3
123	Sound and noisy light: Optical control of phonons in photoswitchable structures. Physical Review B, 2015, 92, .	3.2	2
124	Evidence of Conjugation Enhancement in P3HT/SWNT Mixtures for Organic Photovoltaics. Materials Research Society Symposia Proceedings, 2011, 1286, 56.	0.1	1
125	Resonant behavior in heat transfer across weak molecular interfaces. Journal of Applied Physics, 2013, 114, 234308.	2.5	1
126	Unintended consequences: Why carbonation can dominate in microscale hydration of calcium silicates. Journal of Materials Research, 2015, 30, 2425-2433.	2.6	1



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127	Laser-Induced Cooperative Transition in Molecular Electronic Crystal (Adv. Mater. 39/2021). Advanced Materials, 2021, 33, .	21.0	0