Jeffrey C Grossman

List of Publications by Citations

125 papers	5,353 citations	37 h-index	70 g-index
129 ext. papers	6,820 ext. citations	12 avg, IF	6.58 L-index

#	Paper	IF	Citations
125	Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties. *Physical Review Letters*, **2018**, 120, 145301	7.4	494
124	Exciton radiative lifetimes in two-dimensional transition metal dichalcogenides. *Nano Letters*, **2015**, 15, 2794-800	11.5	409
123	Scalable enhancement of graphene oxide properties by thermally driven phase transformation. *Nature Chemistry*, **2014**, 6, 151-8	17.6	261
122	Multilayer Nanoporous Graphene Membranes for Water Desalination. *Nano Letters*, **2016**, 16, 1027-33	11.5	242
121	Quantifying the potential of ultra-permeable membranes for water desalination. *Energy and Environmental Science*, **2014**, 7, 1134-1141	35.4	227
120	Templated assembly of photoswitches significantly increases the energy-storage capacity of solar thermal fuels. *Nature Chemistry*, **2014**, 6, 441-7	17.6	201
119	Atomistic understandings of reduced graphene oxide as an ultrathin-film nanoporous membrane for separations. *Nature Communications*, **2015**, 6, 8335	17.4	167
118	Ultralow thermal conductivity in all-inorganic halide perovskites. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 8693-8697	11.5	156
117	Optically-controlled long-term storage and release of thermal energy in phase-change materials. *Nature Communications*, **2017**, 8, 1446	17.4	144
116	Water permeability of nanoporous graphene at realistic pressures for reverse osmosis desalination. *Journal of Chemical Physics*, **2014**, 141, 074704	3.9	138
115	Self-Driven Photodetector and Ambipolar Transistor in Atomically Thin GaTe-MoS2 p-n vdW Heterostructure. *ACS Applied Materials & Interfaces*, **2016**, 8, 2533-9	9.5	126
114	Polarity governs atomic interaction through two-dimensional materials. *Nature Materials*, **2018**, 17, 999-1004	41.1	107
113	Atomic Structure and Dynamics of Single Platinum Atom Interactions with Monolayer MoS. *ACS Nano*, **2017**, 11, 3392-3403	16.7	94
112	Machine Learning Enabled Computational Screening of Inorganic Solid Electrolytes for Suppression of Dendrite Formation in Lithium Metal Anodes. *ACS Central Science*, **2018**, 4, 996-1006	16.8	92
111	Optical and Electronic Properties of Two-Dimensional Layered Materials. *Nanophotonics*, **2017**, 6, 479-493	6.3	86
110	Solid-State Solar Thermal Fuels for Heat Release Applications. *Advanced Energy Materials*, **2016**, 6, 1502006	16.8	74
109	Photovoltaic Performance of PbS Quantum Dots Treated with Metal Salts. *ACS Nano*, **2016**, 10, 3382-8	16.7	70

108	Molecularly Engineered Azobenzene Derivatives for High Energy Density Solid-State Solar Thermal Fuels. *ACS Applied Materials & Interfaces*, **2017**, 9, 8679-8687	9.5	68
107	Identifying and Eliminating Emissive Sub-bandgap States in Thin Films of PbS Nanocrystals. *Advanced Materials*, **2015**, 27, 4481-4486	24	68
106	Photon energy storage materials with high energy densities based on diacetylene□azobenzene derivatives. *Journal of Materials Chemistry A*, **2016**, 4, 16157-16165	13	62
105	Atomically Flat Zigzag Edges in Monolayer MoS by Thermal Annealing. *Nano Letters*, **2017**, 17, 5502-5507	11.5	58
104	Correlations from Ion Pairing and the Nernst-Einstein Equation. *Physical Review Letters*, **2019**, 122, 136001	9.4	56
103	Insight on Tricalcium Silicate Hydration and Dissolution Mechanism from Molecular Simulations. *ACS Applied Materials & Interfaces*, **2015**, 7, 14726-33	9.5	56
102	High-efficiency thermoelectrics with functionalized graphene. *Nano Letters*, **2015**, 15, 2830-5	11.5	56
101	Sleep quality, duration, and consistency are associated with better academic performance in college students. *Npj Science of Learning*, **2019**, 4, 16	6	55
100	Photoswitchable Molecular Rings for Solar-Thermal Energy Storage. *Journal of Physical Chemistry Letters*, **2013**, 4, 854-60	6.4	54
99	Solar energy generation in three dimensions. *Energy and Environmental Science*, **2012**, 5, 6880	35.4	52
98	Laser-sculptured ultrathin transition metal carbide layers for energy storage and energy harvesting applications. *Nature Communications*, **2019**, 10, 3112	17.4	48
97	Ionic Highways from Covalent Assembly in Highly Conducting and Stable Anion Exchange Membrane Fuel Cells. *Journal of the American Chemical Society*, **2019**, 141, 18152-18159	16.4	48
96	MoS2 Enhanced T-Phase Stabilization and Tunability Through Alloying. *Journal of Physical Chemistry Letters*, **2016**, 7, 2304-9	6.4	48
95	The Characterization, Stability, and Reactivity of Synthetic Calcium Silicate Surfaces from First Principles. *Journal of Physical Chemistry C*, **2014**, 118, 15214-15219	3.8	45
94	Graph dynamical networks for unsupervised learning of atomic scale dynamics in materials. *Nature Communications*, **2019**, 10, 2667	17.4	43
93	Enhanced Cell Capture on Functionalized Graphene Oxide Nanosheets through Oxygen Clustering. *ACS Nano*, **2017**, 11, 1548-1558	16.7	42
92	Interplay between intrinsic defects, doping, and free carrier concentration in SrTiO3 thin films. *Physical Review B*, **2012**, 85,	3.3	42
91	High Surface Reactivity and Water Adsorption on NiFe2O4 (111) Surfaces. *Journal of Physical Chemistry C*, **2013**, 117, 5678-5683	3.8	40

90	Ultralong 1D Vacancy Channels for Rapid Atomic Migration during 2D Void Formation in Monolayer MoS. *ACS Nano*, **2018**, 12, 7721-7730	16.7	38
89	Role of Structural Defects in the Water Adsorption Properties of MOF-801. *Journal of Physical Chemistry C*, **2018**, 122, 5545-5552	3.8	37
88	Optically-regulated thermal energy storage in diverse organic phase-change materials. *Chemical Communications*, **2018**, 54, 10722-10725	5.8	37
87	Room Temperature Multiferroicity of Charge Transfer Crystals. *ACS Nano*, **2015**, 9, 9373-9	16.7	35
86	Toward Designing Highly Conductive Polymer Electrolytes by Machine Learning Assisted Coarse-Grained Molecular Dynamics. *Chemistry of Materials*, **2020**, 32, 4144-4151	9.6	35
85	Charge separation in nanoscale photovoltaic materials: recent insights from first-principles electronic structure theory. *Journal of Materials Chemistry*, **2010**, 20, 1053-1061		34
84	Rethinking Coal: Thin Films of Solution Processed Natural Carbon Nanoparticles for Electronic Devices. *Nano Letters*, **2016**, 16, 2951-7	11.5	33
83	Origins of the Stokes Shift in PbS Quantum Dots: Impact of Polydispersity, Ligands, and Defects. *ACS Nano*, **2018**, 12, 2838-2845	16.7	32
82	Strain-induced accelerated asymmetric spatial degradation of polymeric vascular scaffolds. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 2640-2645	11.5	31
81	Hierarchical visualization of materials space with graph convolutional neural networks. *Journal of Chemical Physics*, **2018**, 149, 174111	3.9	30
80	Heat Conduction in Nanostructured Materials Predicted by Phonon Bulk Mean Free Path Distribution. *Journal of Heat Transfer*, **2015**, 137,	1.8	29
79	Mesoscale modeling of phononic thermal conductivity of porous Si: interplay between porosity, morphology and surface roughness. *Journal of Computational Electronics*, **2012**, 11, 8-13	1.8	29
78	Photoluminescent Arrays of Nanopatterned Monolayer MoS2. *Advanced Functional Materials*, **2017**, 27, 1703688	15.6	28
77	Conformal Electroplating of Azobenzene-Based Solar Thermal Fuels onto Large-Area and Fiber Geometries. *ACS Applied Materials & Interfaces*, **2016**, 8, 26319-26325	9.5	27
76	Torsional Deformations in Subnanometer MoS Interconnecting Wires. *Nano Letters*, **2016**, 16, 1210-7	11.5	27
75	Revealing the Cluster-Cloud and Its Role in Nanocrystallization. *Advanced Materials*, **2019**, 31, e1808225	24	26
74	Role of solvent-anion charge transfer in oxidative degradation of battery electrolytes. *Nature Communications*, **2019**, 10, 3360	17.4	26
73	Atomic Structure and Dynamics of Defects in 2D MoS Bilayers. *ACS Omega*, **2017**, 2, 3315-3324	3.9	26

72	Origins of hole traps in hydrogenated nanocrystalline and amorphous silicon revealed through machine learning. *Physical Review B*, **2014**, 89,	3.3	26
71	Failing Forward: Stability of Transparent Electrodes Based on Metal Nanowire Networks. *Advanced Materials*, **2021**, 33, e2004356	24	25
70	Striated 2D Lattice with Sub-nm 1D Etch Channels by Controlled Thermally Induced Phase Transformations of PdSe. *Advanced Materials*, **2019**, 31, e1904251	24	24
69	Inorganic Cage Motion Dominates Excited-State Dynamics in 2D-Layered Perovskites (CxH2x+1NH3)2PbI4 (x = 4). *Journal of Physical Chemistry C*, **2019**, 123, 27904-27916	3.8	24
68	Three-dimensional photovoltaics. *Applied Physics Letters*, **2010**, 96, 071902	3.4	24
67	Double-Sided Graphene Oxide Encapsulated Silver Nanowire Transparent Electrode with Improved Chemical and Electrical Stability. *ACS Applied Materials & Interfaces*, **2020**, 12, 17909-17920	9.5	24
66	Atomic Structure and Dynamics of Self-Limiting Sub-Nanometer Pores in Monolayer WS. *ACS Nano*, **2018**, 12, 11638-11647	16.7	24
65	Stress effects on the Raman spectrum of an amorphous material: Theory and experiment on a-Si:H. *Physical Review B*, **2015**, 92,	3.3	23
64	Band Engineering by Controlling vdW Epitaxy Growth Mode in 2D Gallium Chalcogenides. *Advanced Materials*, **2016**, 28, 7375-82	24	23
63	Thermodynamic-driven polychromatic quantum dot patterning for light-emitting diodes beyond eye-limiting resolution. *Nature Communications*, **2020**, 11, 3040	17.4	22
62	Computer calculations across time and length scales in photovoltaic solar cells. *Energy and Environmental Science*, **2016**, 9, 2197-2218	35.4	22
61	Electron-hole separation in ferroelectric oxides for efficient photovoltaic responses. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 6566-6571	11.5	21
60	Mechanism of Thermal Reversal of the (Fulvalene)tetracarbonyldiruthenium Photoisomerization: Toward Molecular Solar-Thermal Energy Storage. *Angewandte Chemie*, **2010**, 122, 9110-9113	3.6	21
59	Atomic structure and defect dynamics of monolayer lead iodide nanodisks with epitaxial alignment on graphene. *Nature Communications*, **2020**, 11, 823	17.4	20
58	Capillary-fed, thin film evaporation devices. *Journal of Applied Physics*, **2020**, 128, 130901	2.5	20
57	Mpemba-Like Behavior in Carbon Nanotube Resonators. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2011**, 42, 3907-3912	2.3	19
56	Catalyst Self-Assembly for Scalable Patterning of Sub 10 nm Ultrahigh Aspect Ratio Nanopores in Silicon. *ACS Applied Materials & Interfaces*, **2016**, 8, 8043-9	9.5	18
55	All-polymeric control of nanoferronics. *Science Advances*, **2015**, 1, e1501264	14.3	18

54	Preserving nanoscale features in polymers during laser induced graphene formation using sequential infiltration synthesis. *Nature Communications*, **2020**, 11, 3636	17.4	18
53	Epitaxial Templating of Two-Dimensional Metal Chloride Nanocrystals on Monolayer Molybdenum Disulfide. *ACS Nano*, **2017**, 11, 6404-6415	16.7	17
52	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	6.4	17
51	Fundamental Insights on Hydration Environment of Boric Acid and Its Role in Separation from Saline Water. *Journal of Physical Chemistry C*, **2020**, 124, 1438-1445	3.8	17
50	Solvent- and Anion-Dependent Li+□O2□Coupling Strength and Implications on the Thermodynamics and Kinetics of Li□O2 Batteries. *Journal of Physical Chemistry C*, **2020**, 124, 4953-4967	3.8	16
49	Unveiling the phonon scattering mechanisms in half-Heusler thermoelectric compounds. *Energy and Environmental Science*, **2020**, 13, 5165-5176	35.4	16
48	Predicting charge density distribution of materials using a local-environment-based graph convolutional network. *Physical Review B*, **2019**, 100,	3.3	15
47	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	9.6	15
46	A 3D-printed molecular ferroelectric metamaterial. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 27204-27210	11.5	14
45	Silver Nanowire Back Electrode Stabilized with Graphene Oxide Encapsulation for Inverted Semitransparent Organic Solar Cells with Longer Lifetime. *ACS Applied Energy Materials*, **2021**, 4, 1431-1441	6.1	12
44	Chemically Driven Interfacial Coupling in Charge-Transfer Mediated Functional Superstructures. *Nano Letters*, **2016**, 16, 2851-9	11.5	11
43	Blue Light Emitting Defective Nanocrystals Composed of Earth-Abundant Elements. *Angewandte Chemie - International Edition*, **2020**, 59, 860-867	16.4	11
42	Highly Conductive and Permeable Nanocomposite Ultrafiltration Membranes Using Laser-Reduced Graphene Oxide. *Nano Letters*, **2021**, 21, 2429-2435	11.5	11
41	Charting lattice thermal conductivity for inorganic crystals and discovering rare earth chalcogenides for thermoelectrics. *Energy and Environmental Science*, **2021**, 14, 3559-3566	35.4	11
40	Natural Carbon By-Products for Transparent Heaters: The Case of Steam-Cracker Tar. *Advanced Materials*, **2019**, 31, e1900331	24	10
39	Laser-Induced Graphene from Polyimide and Polyethersulfone Precursors as a Sensing Electrode in Anodic Stripping Voltammetry. *ACS Applied Materials & Interfaces*, **2020**, 12, 48511-48517	9.5	10
38	Low-frequency Raman spectrum of 2D layered perovskites: Local atomistic motion or superlattice modes?. *Journal of Chemical Physics*, **2020**, 153, 044710	3.9	10
37	Conductive carbonaceous membranes: recent progress and future opportunities. *Journal of Materials Chemistry A*, **2021**, 9, 3270-3289	13	10

36	Ultra-high aspect ratio functional nanoporous silicon via nucleated catalysts. *RSC Advances*, **2017**, 7, 11537-11542	3.7	8
35	Quantitative Mapping of Molecular Substituents to Macroscopic Properties Enables Predictive Design of Oligoethylene Glycol-Based Lithium Electrolytes. *ACS Central Science*, **2020**, 6, 1115-1128	16.8	8
34	Blue Light Emitting Defective Nanocrystals Composed of Earth-Abundant Elements. *Angewandte Chemie*, **2020**, 132, 870-877	3.6	8
33	Charge Density and Redox Potential of LiNiO2 Using Ab Initio Diffusion Quantum Monte Carlo. *Journal of Physical Chemistry C*, **2020**, 124, 5893-5901	3.8	7
32	Optimization of the Thermoelectric Figure of Merit in Crystalline C60 with Intercalation Chemistry. *Nano Letters*, **2016**, 16, 4203-9	11.5	7
31	Importance of Equilibration Method and Sampling for Molecular Dynamics Simulations of Solvent-Lithium-Salt Systems in Lithium-Oxygen Batteries. *Journal of Chemical Theory and Computation*, **2020**, 16, 7255-7266	6.4	7
30	Freestanding Organic Charge-Transfer Conformal Electronics. *Nano Letters*, **2018**, 18, 4346-4354	11.5	7
29	Engineering Efficient p-Type TMD/Metal Contacts Using Fluorographene as a Buffer Layer. *Advanced Electronic Materials*, **2017**, 3, 1600318	6.4	6
28	Bandlike Transport in PbS Quantum Dot Superlattices with Quantum Confinement. *Journal of Physical Chemistry Letters*, **2019**, 10, 3756-3762	6.4	6
27	Tuning the Potential Energy Landscape to Suppress Ostwald Ripening in Surface-Supported Catalyst Systems. *Nano Letters*, **2019**, 19, 8388-8398	11.5	6
26	Kinetics of Sorption in Hygroscopic Hydrogels.. *Nano Letters*, **2022**,	11.5	6
25	Novel nanomaterials for water desalination technology **2013**,		5
24	Functionalized Graphene Superlattice as a Single-Sheet Solar Cell. *Advanced Functional Materials*, **2015**, 25, 5199-5205	15.6	5
23	Transport-Based Modeling of Bubble Nucleation on Gas Evolving Electrodes. *Langmuir*, **2020**, 36, 15112-15118	4	4
22	Charge Transport in Highly Heterogeneous Natural Carbonaceous Materials. *Advanced Functional Materials*, **2019**, 29, 1904283	15.6	3
21	Screening and Understanding Li Adsorption on Two-Dimensional Metallic Materials by Learning Physics and Physics-Simplified Learning. *Jacs Au*, **2021**, 1, 1904-1914		3
20	Design Rules for Transparent Push-Pull Electron Acceptors: A Case Study on Perylenediimide Derivatives. *Journal of Physical Chemistry Letters*, **2020**, 11, 9265-9271	6.4	3
19	High-Pressure-Sintering-Induced Microstructural Engineering for an Ultimate Phonon Scattering of Thermoelectric Half-Heusler Compounds. *Small*, **2021**, 17, e2102045	11	3

18	Nanostructured Bulk-Heterojunction Solar Cells Based on Amorphous Carbon. *ACS Energy Letters*, **2017**, 2, 882-888	20.1	2
17	Emerged Metallicity in Molecular Ferromagnetic Wires. *Nano Letters*, **2021**, 21, 9746-9753	11.5	2
16	Numerical validation of the dusty-gas model for binary diffusion in low aspect ratio capillaries. *Physics of Fluids*, **2021**, 33, 121701	4.4	2
15	Atomic Structure of Dislocations and Grain Boundaries in Two-Dimensional PtSe. *ACS Nano*, **2021**, 15, 16748-16759	16.7	2
14	Emerging Magnetic Interactions in van der Waals Heterostructures. *Nano Letters*, **2020**, 20, 7852-7859	11.5	2
13	Laser-Induced Tar-Mediated Sintering of Metals and Refractory Carbides in Air. *ACS Nano*, **2020**, 14, 10413-10420	16.7	2
12	Atoms to fibers: Identifying novel processing methods in the synthesis of pitch-based carbon fibers.. *Science Advances*, **2022**, 8, eabn1905	14.3	2
11	Nanoporous Silicon-Assisted Patterning of Monolayer MoS2 with Thermally Controlled Porosity: A Scalable Method for Diverse Applications. *ACS Applied Nano Materials*, **2018**, 1, 3548-3556	5.6	1
10	Sound and noisy light: Optical control of phonons in photoswitchable structures. *Physical Review B*, **2015**, 92,	3.3	1
9	Resonant behavior in heat transfer across weak molecular interfaces. *Journal of Applied Physics*, **2013**, 114, 234308	2.5	1
8	Evidence of Conjugation Enhancement in P3HT/SWNT Mixtures for Organic Photovoltaics. *Materials Research Society Symposia Proceedings*, **2011**, 1286, 56		1
7	Oxynitride-Encapsulated Silver Nanowire Transparent Electrode with Enhanced Thermal, Electrical, and Chemical Stability.. *ACS Applied Materials & Interfaces*, **2022**, 14, 4423-4433	9.5	1
6	Laser-Induced Cooperative Transition in Molecular Electronic Crystal. *Advanced Materials*, **2021**, 33, e2103000	24	1
5	Unintended consequences: Why carbonation can dominate in microscale hydration of calcium silicates. *Journal of Materials Research*, **2015**, 30, 2425-2433	2.5	0
4	Upgrading carbonaceous materials: Coal, tar, pitch, and beyond. *Matter*, **2022**, 5, 430-447	12.7	0
3	Adsorption-based membranes for air separation using transition metal oxides. *Nanoscale Advances*, **2021**, 3, 4502-4512	5.1	0
2	Laser-Induced Cooperative Transition in Molecular Electronic Crystal (Adv. Mater. 39/2021). *Advanced Materials*, **2021**, 33, 2170309	24	
1	Cyclobutene based macrocycles. *Materials Chemistry Frontiers*, **2020**, 4, 3529-3538	7.8	