Alan J H Mcgaughey

List of Publications by Year
in descending order

64 papers	5,447 citations	126907 33 h-index	114465 63 g-index
64 all docs	64 docs citations	64 times ranked	5947 citing authors

#	Article	IF	Citations
1	Finite-temperature force constants are essential for accurately predicting the thermal conductivity of rutile <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Materials, 2022, 6, .	2.4	3
2	Reducing the uncertainty caused by the laser spot radius in frequency-domain thermoreflectance measurements of thermal properties. Review of Scientific Instruments, 2022, 93, 023001.	1.3	4
3	Highly Negative Poissonâ€™s Ratio in Thermally Conductive Covalent Organic Frameworks. ACS Nano, 2022, 16, 2843-2851.	14.6	17
4	Hybridization from Guestâ€"Host Interactions Reduces the Thermal Conductivity of Metalâ€"Organic Frameworks. Journal of the American Chemical Society, 2022, 144, 3603-3613.	13.7	23
5	XGBoost model for electrocaloric temperature change prediction in ceramics. Npj Computational Materials, 2022, 8, .	8.7	15
6	Thermally conductive ultra-low-k dielectric layers based on two-dimensional covalent organic frameworks. Nature Materials, 2021, 20, 1142-1148.	27.5	158
7	Nanoconfinement between Graphene Walls Suppresses the Near-Wall Diffusion of the Ionic Liquid [BMIM][PF6]. Journal of Physical Chemistry B, 2021, 125, 4527-4535.	2.6	8
8	Universal Model for Predicting the Thermal Boundary Conductance of a Multilayered-Metalâ€"Dielectric Interface. Physical Review Applied, 2021, 15, .	3.8	3
9	Observation of reduced thermal conductivity in a metal-organic framework due to the presence of adsorbates. Nature Communications, 2020, 11, 4010.	12.8	97
10	Fullerene rotational dynamics generate disordered configurations that suppress thermal conductivity in superatomic crystals. Nanoscale Horizons, 2020, 5, 1524-1529.	8.0	7
11	Mean Free Path Suppression of Low-Frequency Phonons in SiGe Nanowires. Nano Letters, 2020, 20, 8384-8391.	9.1	12
12	Assessing the impact of disjoining pressure on thin-film evaporation with atomistic simulation and kinetic theory. Applied Physics Letters, 2020, 116, .	3.3	12
13	Deviceâ€level thermodynamic model for an electrocaloric cooler. International Journal of Energy Research, 2020, 44, 5343-5359.	4.5	12
14	Phonon confinement and transport in ultrathin films. Physical Review B, 2020, 101, .	3.2	17
15	Uncertainty quantification in first-principles predictions of phonon properties and lattice thermal conductivity. Physical Review Materials, 2020, 4, .	2.4	2
16	Mapping phonon modes from reduced-dimensional to bulk systems. Journal of Applied Physics, 2019, 126, 144302.	2.5	2
17	Uncertainty Quantification in First-Principles Predictions of Harmonic Vibrational Frequencies of Molecules and Molecular Complexes. Journal of Physical Chemistry C, 2019, 123, 4072-4084.	3.1	16
18	Chemical Reactions Impede Thermal Transport Across Metal/Î²-Ga₂O₃ Interfaces. Nano Letters, 2019, 19, 8533-8538.	9.1	28

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19	Thermal Transport in Disordered Materials. Nanoscale and Microscale Thermophysical Engineering, 2019, 23, 81-116.	2.6	66
20	Phonon properties and thermal conductivity from first principles, lattice dynamics, and the Boltzmann transport equation. Journal of Applied Physics, 2019, 125, .	2.5	141
21	Transient Mass and Thermal Transport during Methane Adsorption into the Metalâ€“Organic Framework HKUST-1. ACS Applied Materials & Interfaces, 2018, 10, 2400-2406.	8.0	46
22	Contributions of different degrees of freedom to thermal transport in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math> molecular crystal. Physical Review B, 2018, 97, .	3.2	11
23	Spontaneous Electronic Band Formation and Switchable Behaviors in a Phase-Rich Superatomic Crystal. Journal of the American Chemical Society, 2018, 140, 15601-15605.	13.7	17
24	Materials enabling nanofluidic flow enhancement. MRS Bulletin, 2017, 42, 273-277.	3.5	4
25	Thermal conductance of graphene/hexagonal boron nitride heterostructures. Journal of Applied Physics, 2017, 121, 115103.	2.5	19
26	Near-field radiative heat transfer in graphene plasmonic nanodisk dimers. Physical Review B, 2017, 96, .	3.2	25
27	Plasmonic thermal transport in graphene nanodisk waveguides. Physical Review B, 2017, 96, .	3.2	13
28	Phonon-boundary scattering in nanoporous silicon films: Comparison of Monte Carlo techniques. Journal of Applied Physics, 2017, 122, .	2.5	38
29	Orientational order controls crystalline andÂamorphous thermal transport in superatomicÂcrystals. Nature Materials, 2017, 16, 83-88.	27.5	94
30	Effect of pore size and shape on the thermal conductivity of metal-organic frameworks. Chemical Science, 2017, 8, 583-589.	7.4	120
31	Energy barriers for dipole moment flipping in PVDF-related ferroelectric polymers. Journal of Chemical Physics, 2016, 144, 014901.	3.0	33
32	Thermal transport by phonons and electrons in aluminum, silver, and gold from first principles. Physical Review B, 2016, 93, .	3.2	166
33	Thermal conductance of superlattice junctions. AIP Advances, 2015, 5, 053205.	1.3	11
34	Strongly anisotropic in-plane thermal transport in single-layer black phosphorene. Scientific Reports, 2015, 5, 8501.	3.3	463
35	Effect of exchangeâ€“correlation on first-principles-driven lattice thermal conductivity predictions of crystalline silicon. Computational Materials Science, 2015, 110, 115-120.	3.0	74
36	Release and transfer of large-area ultra-thin PDMS. , 2014, , .		3

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37	Origins of thermal conductivity changes in strained crystals. Physical Review B, 2014, 90, .	3.2	84
38	Electrocaloric characterization of a poly(vinylidene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 707 Td (fluoride-trifluoroethylene-chlorofluoro Letters, 2014, 105, .	3.3	27
39	Thermal conductivity accumulation in amorphous silica and amorphous silicon. Physical Review B, 2014, 89, .	3.2	214
40	Design and modeling of a fluid-based micro-scale electrocaloric refrigeration system. International Journal of Heat and Mass Transfer, 2014, 72, 559-564.	4.8	68
41	Thermal conductivity of compound semiconductors: Interplay of mass density and acoustic-optical phonon frequency gap. Journal of Applied Physics, 2014, 116, .	2.5	38
42	Coupling of Organic and Inorganic Vibrational States and Their Thermal Transport in Nanocrystal Arrays. Journal of Physical Chemistry C, 2014, 118, 7288-7295.	3.1	68
43	TFOx: A versatile kinetic Monte Carlo program for simulations of island growth in three dimensions. Computational Materials Science, 2014, 91, 292-302.	3.0	9
44	PREDICTING PHONON PROPERTIES FROM EQUILIBRIUM MOLECULAR DYNAMICS SIMULATIONS. Annual Review of Heat Transfer, 2014, 17, 49-87.	1.0	81
45	Predicting alloy vibrational mode properties using lattice dynamics calculations, molecular dynamics simulations, and the virtual crystal approximation. Journal of Applied Physics, 2013, 114, .	2.5	64
46	Surface chemistry mediates thermal transport in three-dimensional nanocrystal arrays. Nature Materials, 2013, 12, 410-415.	27.5	218
47	Broadband phonon mean free path contributions to thermal conductivity measured using frequency domain thermoreflectance. Nature Communications, 2013, 4, 1640.	12.8	479
48	Phonon transport in periodic silicon nanoporous films with feature sizes greater than 100 nm. Physical Review B, 2013, 87, .	3.2	127
49	Disruption of superlattice phonons by interfacial mixing. Physical Review B, 2013, 88, .	3.2	50
50	Nanostructure thermal conductivity prediction by Monte Carlo sampling of phonon free paths. Applied Physics Letters, 2012, 100, 061911.	3.3	76
51	<i>Ab initio</i>atomistic thermodynamics study of the early stages of Cu(100) oxidation. Physical Review B, 2012, 86, .	3.2	42
52	Gas Diffusion, Energy Transport, and Thermal Accommodation in Singleâ€Walled Carbon Nanotube Aerogels. Advanced Functional Materials, 2012, 22, 5251-5258.	14.9	95
53	Atomistic simulations of copper oxidation and Cu/Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O interfaces using charge-optimized many-body potentials. Physical Review B, 2011, 84, .	3.2	68
54	Size-dependent model for thin film and nanowire thermal conductivity. Applied Physics Letters, 2011, 99, .	3.3	126

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55	Energetics and kinetics of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>c</mml:mi></mml:mrow></mml:math>(<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf		