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	Reassessing Fast Water Transport Through Carbon Nanotubes. Nano Letters, 2008, 8, 2788-2793.	9.1	599
2	Broadband phonon mean free path contributions to thermal conductivity measured using frequency domain thermoreflectance. Nature Communications, 2013, 4, 1640.	12.8	479
3	Strongly anisotropic in-plane thermal transport in single-layer black phosphorene. Scientific Reports, 2015, 5, 8501.	3.3	463
4	Water Flow in Carbon Nanotubes: Transition to Subcontinuum Transport. Physical Review Letters, 2009, 102, 184502.	7.8	402
5	Predicting phonon dispersion relations and lifetimes from the spectral energy density. Physical Review B, 2010, 81, .	3.2	285
6	Surface chemistry mediates thermal transport in three-dimensional nanocrystal arrays. Nature Materials, 2013, 12, 410-415.	27.5	218
7	Thermal conductivity accumulation in amorphous silica and amorphous silicon. Physical Review B, 2014, 89, .	3.2	214
8	Thermal transport by phonons and electrons in aluminum, silver, and gold from first principles. Physical Review B, 2016, 93, .	3.2	166
9	Thermally conductive ultra-low-k dielectric layers based on two-dimensional covalent organic frameworks. Nature Materials, 2021, 20, 1142-1148.	27.5	158
10	Phonon properties and thermal conductivity from first principles, lattice dynamics, and the Boltzmann transport equation. Journal of Applied Physics, 2019, 125, .	2.5	141
11	Pressure-driven water flow through carbon nanotubes: Insights from molecular dynamics simulation. International Journal of Thermal Sciences, 2010, 49, 281-289.	4.9	140
12	Thermal conductivity and phonon transport in empty and water-filled carbon nanotubes. Physical Review B, 2010, 81, .	3.2	133
13	Phonon transport in periodic silicon nanoporous films with feature sizes greater than 100 nm. Physical Review B, 2013, 87, .	3.2	127
14	Size-dependent model for thin film and nanowire thermal conductivity. Applied Physics Letters, 2011, 99, .	3.3	126
15	Effect of pore size and shape on the thermal conductivity of metal-organic frameworks. Chemical Science, 2017, 8, 583-589.	7.4	120
16	Observation of reduced thermal conductivity in a metal-organic framework due to the presence of adsorbates. Nature Communications, 2020, 11, 4010.	12.8	97
17	Gas Diffusion, Energy Transport, and Thermal Accommodation in Singleâ€Walled Carbon Nanotube Aerogels. Advanced Functional Materials, 2012, 22, 5251-5258.	14.9	95
18	Orientational order controls crystalline andÂamorphous thermal transport in superatomicÂcrystals. Nature Materials, 2017, 16, 83-88.	27.5	94

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19	Predicting the thermal conductivity of inorganic and polymeric glasses: The role of anharmonicity. Journal of Applied Physics, 2009, 105, .	2.5	88
20	Origins of thermal conductivity changes in strained crystals. Physical Review B, 2014, 90, .	3.2	84
21	PREDICTING PHONON PROPERTIES FROM EQUILIBRIUM MOLECULAR DYNAMICS SIMULATIONS. Annual Review of Heat Transfer, 2014, 17, 49-87.	1.0	81
22	Nanostructure thermal conductivity prediction by Monte Carlo sampling of phonon free paths. Applied Physics Letters, 2012, 100, 061911.	3.3	76
23	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
24	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
25	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
26	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
27	Thermal Transport in Disordered Materials. Nanoscale and Microscale Thermophysical Engineering, 2019, 23, 81-116.	2.6	66
28	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
29	Disruption of superlattice phonons by interfacial mixing. Physical Review B, 2013, 88, .	3.2	50
30	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
31	<i>Ab initio</i>atomistic thermodynamics study of the early stages of Cu(100) oxidation. Physical Review B, 2012, 86, .	3.2	42
32	Thermal conductivity of compound semiconductors: Interplay of mass density and acoustic-optical phonon frequency gap. Journal of Applied Physics, 2014, 116, .	2.5	38
33	Phonon-boundary scattering in nanoporous silicon films: Comparison of Monte Carlo techniques. Journal of Applied Physics, 2017, 122, .	2.5	38
34	Energy barriers for dipole moment flipping in PVDF-related ferroelectric polymers. Journal of Chemical Physics, 2016, 144, 014901.	3.0	33
35	Chemical Reactions Impede Thermal Transport Across Metal/Î²-Ga₂O₃ Interfaces. Nano Letters, 2019, 19, 8533-8538.	9.1	28
36	Electrocaloric characterization of a poly(vinylidene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 67 Td (fluoride-trifluoroethylene-chlorofluoroe Letters, 2014, 105, .	3.3	27

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37	Energetics of oxygen embedment into unreconstructed and reconstructed Cu(1 0 0) surfaces: Density functional theory calculations. Surface Science, 2009, 603, 3404-3409.	1.9	26
38	Role of sub-surface oxygen in Cu(100) oxidation. Surface Science, 2010, 604, 1425-1431.	1.9	25
39	Near-field radiative heat transfer in graphene plasmonic nanodisk dimers. Physical Review B, 2017, 96, .	3.2	25
40	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
41	Thermal conductance of graphene/hexagonal boron nitride heterostructures. Journal of Applied Physics, 2017, 121, 115103.	2.5	19
42	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 ETQq0 0 0 rgBT /Overlock 10 Tf 50 552		

#	ARTICLE	IF	CITATIONS
55	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
56	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
57	Fullerene rotational dynamics generate disordered configurations that suppress thermal conductivity in superatomic crystals. Nanoscale Horizons, 2020, 5, 1524-1529.	8.0	7
58	Materials enabling nanofluidic flow enhancement. MRS Bulletin, 2017, 42, 273-277.	3.5	4
59	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
60	Release and transfer of large-area ultra-thin PDMS. , 2014, , .		3
61	Universal Model for Predicting the Thermal Boundary Conductance of a Multilayered-Metalâ€“Dielectric Interface. Physical Review Applied, 2021, 15, .	3.8	3
62	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
63	Mapping phonon modes from reduced-dimensional to bulk systems. Journal of Applied Physics, 2019, 126, 144302.	2.5	2
64	Uncertainty quantification in first-principles predictions of phonon properties and lattice thermal conductivity. Physical Review Materials, 2020, 4, .	2.4	2