JesÃºs Carrete

List of Publications by Year
in descending order

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128 papers	8,073 citations	61984 43 h-index	49909 87 g-index
128 all docs	128 docs citations	128 times ranked	7306 citing authors

#	Article	IF	Citations
1	ShengBTE: A solver of the Boltzmann transport equation for phonons. Computer Physics Communications, 2014, 185, 1747-1758.	7.5	1,931
2	BoltzTraP2, a program for interpolating band structures and calculating semi-classical transport coefficients. Computer Physics Communications, 2018, 231, 140-145.	7.5	730
3	Phonon thermal transport in strained and unstrained graphene from first principles. Physical Review B, 2014, 89, .	3.2	319
4	Thermal conductivity and phonon linewidths of monolayer MoS2 from first principles. Applied Physics Letters, 2013, 103, .	3.3	273
5	Low thermal conductivity and triaxial phononic anisotropy of SnSe. Applied Physics Letters, 2014, 105, .	3.3	226
6	Physically founded phonon dispersions of few-layer materials and the case of borophene. Materials Research Letters, 2016, 4, 204-211.	8.7	216
7	Finding Unprecedentedly Low-Thermal-Conductivity Half-Heusler Semiconductors via High-Throughput Materials Modeling. Physical Review X, 2014, 4, .	8.9	210
8	almaBTE : A solver of the spaceâ€“time dependent Boltzmann transport equation for phonons in structured materials. Computer Physics Communications, 2017, 220, 351-362.	7.5	193
9	Strong enhancement of phonon scattering through nanoscale grains in lead sulfide thermoelectrics. NPG Asia Materials, 2014, 6, e108-e108.	7.9	140
10	Molecular Dynamics Simulation of the Structure and Dynamics of Waterâ€“1-Alkyl-3-methylimidazolium Ionic Liquid Mixtures. Journal of Physical Chemistry B, 2011, 115, 6995-7008.	2.6	127
11	Nanograined Halfâ€Heusler Semiconductors as Advanced Thermoelectrics: An Ab Initio Highâ€Throughput Statistical Study. Advanced Functional Materials, 2014, 24, 7427-7432.	14.9	117
12	Unexpected High-Temperature Stability of Î²-Zn₄Sb₃ Opens the Door to Enhanced Thermoelectric Performance. Journal of the American Chemical Society, 2014, 136, 1497-1504.	13.7	115
13	How Chemical Composition Alone Can Predict Vibrational Free Energies and Entropies of Solids. Chemistry of Materials, 2017, 29, 6220-6227.	6.7	103
14	Temperature and Thickness Dependences of the Anisotropic Inâ€Plane Thermal Conductivity of Black Phosphorus. Advanced Materials, 2017, 29, 1603756.	21.0	99
15	MD Simulations of the Formation of Stable Clusters in Mixtures of Alkaline Salts and Imidazolium-Based Ionic Liquids. Journal of Physical Chemistry B, 2013, 117, 3207-3220.	2.6	92
16	Effect of Temperature and Cationic Chain Length on the Physical Properties of Ammonium Nitrate-Based Protic Ionic Liquids. Journal of Physical Chemistry B, 2012, 116, 11302-11312.	2.6	87
17	Solvation of Lithium Salts in Protic Ionic Liquids: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2014, 118, 761-770.	2.6	87
18	Effect of nitrogen and vacancy defects on the thermal conductivity of diamond: Anab initioGreen's function approach. Physical Review B, 2014, 90, .	3.2	87

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19	Mixtures of protic ionic liquids and molecular cosolvents: A molecular dynamics simulation. Journal of Chemical Physics, 2014, 140, 214502.	3.0	78
20	Materials Screening for the Discovery of New Half-Heuslers: Machine Learning versus ab Initio Methods. Journal of Physical Chemistry B, 2018, 122, 625-632.	2.6	78
21	Solvation of molecular cosolvents and inorganic salts in ionic liquids: A review of molecular dynamics simulations. Journal of Molecular Liquids, 2015, 210, 178-188.	4.9	76
22	Superdiffusive heat conduction in semiconductor alloys. I. Theoretical foundations. Physical Review B, 2015, 91, .	3.2	75
23	Twisting phonons in complex crystals with quasi-one-dimensional substructures. Nature Communications, 2015, 6, 6723.	12.8	75
24	Surface roughness and thermal conductivity of semiconductor nanowires: Going below the Casimir limit. Physical Review B, 2011, 84, .	3.2	74
25	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. Computational Materials Science, 2018, 152, 134-145.	3.0	72
26	Anomalous pressure dependence of thermal conductivities of large mass ratio compounds. Physical Review B, 2015, 91, .	3.2	71
27	Exceptionally Strong Phonon Scattering by B Substitution in Cubic SiC. Physical Review Letters, 2017, 119, 075902.	7.8	68
28	Liquidâ€“solidâ€“liquid phase transition hysteresis loops in the ionic conductivity of ten imidazolium-based ionic liquids. Fluid Phase Equilibria, 2012, 320, 1-10.	2.5	65
29	Ti-decorated zigzag graphene nanoribbons for hydrogen storage. A van der Waals-corrected density-functional study. International Journal of Hydrogen Energy, 2015, 40, 4960-4968.	7.1	65
30	Ab initiostudy of the effect of vacancies on the thermal conductivity of boron arsenide. Physical Review B, 2016, 94, .	3.2	65
31	An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOWâ€”AAPL Automatic Anharmonic Phonon Library. Npj Computational Materials, 2017, 3, .	8.7	65
32	High-Throughput Computation of Thermal Conductivity of High-Temperature Solid Phases: The Case of Oxide and Fluoride Perovskites. Physical Review X, 2016, 6, .	8.9	61
33	Anomalous thermal conductivity and suppression of negative thermal expansion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ScF</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2016, 94, .	3.2	61
34	Molecular Dynamics Simulations of the Structural and Thermodynamic Properties of Imidazolium-Based Ionic Liquid Mixtures. Journal of Physical Chemistry B, 2011, 115, 11170-11182.	2.6	58
35	Molecular dynamics simulations of the structure of the grapheneâ€“ionic liquid/alkali salt mixtures interface. Physical Chemistry Chemical Physics, 2014, 16, 13271-13278.	2.8	58
36	Influence of the optical-acoustic phonon hybridization on phonon scattering and thermal conductivity. Physical Review B, 2016, 93, .	3.2	55

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37	How does lithium nitrate dissolve in a protic ionic liquid?. Journal of Molecular Liquids, 2015, 205, 16-21.	4.9	53
38	Ab initiostudy of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>5</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>transition	3.2	49
39	Ab initio phonon scattering by dislocations. Physical Review B, 2017, 95, .	3.2	49
40	Phonon thermal transport in 2H, 4H and 6H silicon carbide from first principles. Materials Today Physics, 2017, 1, 31-38.	6.0	48
41	Surfactant Self-Assembly Nanostructures in Protic Ionic Liquids. Journal of Physical Chemistry B, 2011, 115, 8145-8154.	2.6	47
42	Pseudolattice theory of charge transport in ionic solutions: Corresponding states law for the electric conductivity. Fluid Phase Equilibria, 2010, 298, 280-286.	2.5	46
43	Ultrahigh Thermal Conductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î‚</mml:mi></mml:math> -Phase Tantalum Nitride. Physical Review Letters, 2021, 126, 115901.	7.8	46
44	Structural, magnetic, and electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ni</mml:mtext></mml:mrow><mml:mi>n</mml:mi></mml:msub> xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mi>n</mml:mi></mml:msub> xmlns:mml="http://www.w3.org/1998/Math/MathML" displa. Physical Review B, 2010, 81, .	3.2	44
45	Cross-plane heat conduction in thin films with ab-initio phonon dispersions and scattering rates. Applied Physics Letters, 2016, 108, .	3.3	44
46	Structural Complexity and Phonon Physics in 2D Arsenenes. Journal of Physical Chemistry Letters, 2017, 8, 1375-1380.	4.6	41
47	Unraveling the dominant phonon scattering mechanism in the thermoelectric compound ZrNiSn. Journal of Materials Chemistry A, 2016, 4, 15940-15944.	10.3	40
48	An investigation of the structural properties of Li and Na fast ion conductors using high-throughput bond-valence calculations and machine learning. Journal of Applied Crystallography, 2019, 52, 148-157.	4.5	39
49	Nanostructure of mixtures of protic ionic liquids and lithium salts: effect of alkyl chain length. Physical Chemistry Chemical Physics, 2015, 17, 5298-5307.	2.8	37
50	First-principles quantitative prediction of the lattice thermal conductivity in random semiconductor alloys: The role of force-constant disorder. Physical Review B, 2018, 98, .	3.2	36
51	Re-entrant phase behavior for systems with competition between phase separation and self-assembly. Journal of Chemical Physics, 2011, 134, 104905.	3.0	34
52	Dynamical Properties of Alcohol + 1-Hexyl-3-methylimidazolium Ionic Liquid Mixtures: A Computer Simulation Study. Journal of Physical Chemistry B, 2011, 115, 15313-15322.	2.6	33
53	What will freestanding borophene nanoribbons look like? An analysis of their possible structures, magnetism and transport properties. Physical Chemistry Chemical Physics, 2017, 19, 1054-1061.	2.8	32
54	Pseudolattice Theory of the Surface Tension of Ionic Liquidâ^'Water Mixtures. Journal of Physical Chemistry B, 2009, 113, 12500-12505.	2.6	30

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55	Combined treatment of phonon scattering by electrons and point defects explains the thermal conductivity reduction in highly-doped Si. Journal of Materials Chemistry A, 2020, 8, 1273-1278.	10.3	30
56	The Effect of Janus Asymmetry on Thermal Transport in SnSSe. Journal of Physical Chemistry C, 2020, 124, 17476-17484.	3.1	30
57	Magnetism of substitutional Fe impurities in graphene nanoribbons. Journal of Chemical Physics, 2011, 134, 024704.	3.0	29
58	Ultralow lattice thermal conductivity in topological insulator TlBiSe2. Applied Physics Letters, 2016, 108, .	3.3	29
59	Shortcomings of meta-GGA functionals when describing magnetism. Physical Review B, 2020, 102, .	3.2	27
60	Al enhances the H<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>storage capacity of graphene at nanoribbon borders but not at central sites: A study using nonlocal van der Waals density functionals. Physical Review B, 2012, 85, .	3.2	25
61	Investigation of the Local Structure of Mixtures of an Ionic Liquid with Polar Molecular Species through Molecular Dynamics: Cluster Formation and Angular Distributions. Journal of Physical Chemistry B, 2012, 116, 5941-5950.	2.6	25
62	Phonon Scattering by Dislocations in GaN. ACS Applied Materials & Interfaces, 2019, 11, 8175-8181.	8.0	25
63	Thermoelectric Properties of Hybrid Organicâ€“Inorganic Superlattices. Journal of Physical Chemistry C, 2012, 116, 10881-10886.	3.1	24
64	A theoretical model of the thermoelectric properties of SnSxSe1â^'x and how to further enhance its thermoelectric performance. Journal of Applied Physics, 2019, 126, .	2.5	24
65	Molecular hydrogen uptake by zigzag graphene nanoribbons doped with early 3d transition-metal atoms. International Journal of Hydrogen Energy, 2013, 38, 8872-8880.	7.1	22
66	Thermal transport through Ge-rich Ge/Si superlattices grown on Ge(0â€‰0â€‰1). Journal Physics D: Applied Physics, 2018, 51, 014001.	2.8	22
67	Phonon transport unveils the prevalent point defects in GaN. Physical Review Materials, 2018, 2, .	2.4	22
68	Influence of point defects on the thermal conductivity in FeSi. Physical Review B, 2018, 97, .	3.2	21
69	How dopants limit the ultrahigh thermal conductivity of boron arsenide: a first principles study. Npj Computational Materials, 2021, 7, .	8.7	21
70	Independently tuning the power factor and thermal conductivity of SnSe via Ag2S addition and nanostructuring. Journal of Materials Chemistry A, 2018, 6, 7959-7966.	10.3	20
71	Microstructure investigations and thermoelectrical properties of an N-type magnesiumâ€“siliconâ€“tin alloy sintered from a gas-phase atomized powder. Acta Materialia, 2015, 96, 437-451.	7.9	19
72	Anomalously large lattice thermal conductivity in metallic tungsten carbide and its origin in the electronic structure. Materials Today Physics, 2020, 13, 100214.	6.0	19

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73	Thermal Conductivity of Ionic Liquids: A Pseudolattice Approach. Journal of Physical Chemistry C, 2012, 116, 1265-1273.	3.1	18
74	Quantum Self-Consistent Ab-Initio Lattice Dynamics. Computer Physics Communications, 2021, 263, 107945.	7.5	18
75	Theoretical model for moisture adsorption on ionic liquids: A modified Brunauerâ€"Emmetâ€"Teller isotherm approach. Fluid Phase Equilibria, 2011, 301, 118-122.	2.5	17
76	Resonant phonon scattering in semiconductors. Journal of Materials Chemistry C, 2018, 6, 4691-4697.	5.5	17
77	Ab initio lattice thermal conductivity of bulk and thin-film Î±-Al2O3. MRS Communications, 2018, 8, 1119-1123.	1.8	17
78	Phonon transport across crystal-phase interfaces and twin boundaries in semiconducting nanowires. Nanoscale, 2019, 11, 16007-16016.	5.6	17
79	Thermal Resistance of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>Ga</mml:mi><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> / <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>Al</mml:mi><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> Graded Interfaces. Physical Review	3.8	17
80	Localized dimers drive strong anharmonicity and low lattice thermal conductivity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Zn</mml:mi><mml:msub><mml:mi>Se</mml:mi><mml:m Physical Review B, 2020, 102, .	3.2	17
81	A Differentiable Neural-Network Force Field for Ionic Liquids. Journal of Chemical Information and Modeling, 2022, 62, 88-101.	5.4	17
82	Influence of Antisite Defects on the Thermoelectric Properties of Fe₂VAl. Nanoscale and Microscale Thermophysical Engineering, 2017, 21, 237-246.	2.6	16
83	Machine-learning Prediction of Infrared Spectra of Interstellar Polycyclic Aromatic Hydrocarbons. Astrophysical Journal, 2020, 902, 100.	4.5	16
84	Atomistic origin of glass-like Zn4Sb3 thermal conductivity. Applied Physics Letters, 2013, 103, 103902.	3.3	15
85	Thermoelectric properties of the SnS monolayer: Fully <i>ab initio</i> and accelerated calculations. Journal of Applied Physics, 2021, 130, .	2.5	15
86	Human Immune Protein C1q Selectively Disaggregates Carbon Nanotubes. Nano Letters, 2017, 17, 3409-3415.	9.1	14
87	Predictive Design and Experimental Realization of InAs/GaAs Superlattices with Tailored Thermal Conductivity. Journal of Physical Chemistry C, 2018, 122, 4054-4062.	3.1	14
88	Vibrational Properties of Metastable Polymorph Structures by Machine Learning. Journal of Chemical Information and Modeling, 2018, 58, 2460-2466.	5.4	14
89	Nonextensive statistical mechanics of ionic solutions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 370, 405-412.	2.1	13
90	Complex Network Analysis in Socioeconomic Models. Dynamic Modeling and Econometrics in Economics and Finance, 2015, , 209-245.	0.5	13

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91	Molecular-dynamics prediction of the thermal conductivity of thin InP nanowires: Similarities to Si. Physical Review B, 2009, 80, .	3.2	12
92	Role of force-constant difference in phonon scattering by nano-precipitates in PbTe. Journal of Applied Physics, 2015, 118, .	2.5	12
93	Basal-plane thermal conductivity of nanocrystalline and amorphized thin germanane. Applied Physics Letters, 2016, 109, 131907.	3.3	11
94	Density Functional Study of Charge Transfer at the Graphene/Ionic Liquid Interface. Journal of Physical Chemistry C, 2018, 122, 15070-15077.	3.1	11
95	Parameter-free model to estimate thermal conductivity in nanostructured materials. Physical Review B, 2019, 100, .	3.2	11
96	Prediction of phonon thermal transport in thin GaAs, InAs and InP nanowires by molecular dynamics simulations: influence of the interatomic potential. Nanotechnology, 2011, 22, 185704.	2.6	10
97	Glass-like thermal conductivity in nanostructures of a complex anisotropic crystal. Physical Review B, 2017, 96, .	3.2	10
98	The AFLOW Fleet for Materials Discovery. , 2018, , 1-28.		9
99	Coupling of Spinons with Defects and Phonons in the Spin Chain Compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ca</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub><mn Physical Review Letters, 2019, 122, 185901.	7.8	9
100	Effect of local chemistry and structure on thermal transport in doped GaAs. Physical Review Materials, 2019, 3, .	2.4	9
101	Borophene vs. graphene interfaces: Tuning the electric double layer in ionic liquids. Journal of Molecular Liquids, 2020, 303, 112647.	4.9	8
102	Anisotropic Thermal Conductivity in Few-Layer and Bulk Titanium Trisulphide from First Principles. Nanomaterials, 2020, 10, 704.	4.1	8
103	Optimisation of the thermoelectric efficiency of zirconium trisulphide monolayers through unixial and biaxial strain. Nanoscale Advances, 2020, 2, 5352-5361.	4.6	8
104	High-throughput study of the static dielectric constant at high temperatures in oxide and fluoride cubic perovskites. Physical Review Materials, 2020, 4, .	2.4	8
105	A density-functional study of the structures and electronic properties of neutral, anionic, and endohedrally doped InxPx clusters. Journal of Chemical Physics, 2009, 131, 074504.	3.0	7
106	Growth, charge and thermal transport of flowered graphene. Carbon, 2020, 161, 259-268.	10.3	7
107	Nonequilibrium nanothermodynamics. Physical Review E, 2008, 77, 022102.	2.1	6
108	Optimizing phonon scattering by nanoprecipitates in lead chalcogenides. Applied Physics Letters, 2016, 108, 113901.	3.3	6

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109	Understanding Phonon Scattering by Nanoprecipitates in Potassium-Doped Lead Chalcogenides. ACS Applied Materials & Interfaces, 2017, 9, 3686-3693.	8.0	6
110	Revisiting the thermal conductivity of Si, Ge and diamond from first principles: roles of atomic mass and interatomic potential. Journal of Physics Condensed Matter, 2021, 33, 285702.	1.8	6
111	Strain-tunable lattice thermal conductivity of the Janus PtSTe monolayer. Journal of Physics Condensed Matter, 2022, 34, 015303.	1.8	6
112	Chemical trends in the high thermoelectric performance of the pyrite-type dichalcogenides <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZnS</mml:mi><mml:mn>2</mml:mn></mml:msub><mml , and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CdSe</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2022, 105, .	3.2	6
113	A density-functional study of the vertical ionization potentials of the cluster Mn13. Journal of Chemical Physics, 2009, 131, 046101.	3.0	5
114	Influence of the addition of Half-Heusler nanoparticles on the thermoelectrical properties of an N-type magnesiumâ€“siliconâ€“tin alloy. Scripta Materialia, 2015, 104, 5-8.	5.2	5
115	Effects of doping substitutions on the thermal conductivity of half-Heusler compounds. Physical Review B, 2021, 103, .	3.2	5
116	Microcanonical equations obtained from the Tsallis entropy. Physica A: Statistical Mechanics and Its Applications, 2008, 387, 6752-6758.	2.6	4
117	Twisted bilayer graphene as a linear nanoactuator. Physical Review B, 2020, 102, .	3.2	4
118	The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812.		4
119	Accurate firstâ€principles treatment of the highâ€temperature cubic phase of hafnia. Physica Status Solidi - Rapid Research Letters, 0, , .	2.4	4
120	Electronic properties of pure and p-type doped hexagonal sheets and zigzag nanoribbons of InP. Journal of Physics Condensed Matter, 2013, 25, 085506.	1.8	3
121	Tunable gap in stable arsenene nanoribbons opens the door to electronic applications. RSC Advances, 2019, 9, 11818-11823.	3.6	3
122	Using nanotubes to study the phonon spectrum of two-dimensional materials. Physical Chemistry Chemical Physics, 2019, 21, 5215-5223.	2.8	3
123	Pseudolattice Theory of Ionic Liquids. , 2011, , .		2
124	Structural, magnetic, and vibrational properties of stoichiometric clusters of <scp>C</scp>r<scp>N</scp>. International Journal of Quantum Chemistry, 2015, 115, 523-528.	2.0	2
125	Influence of Onion-like Carbonaceous Particles on the Aggregation Process of Hydrocarbons. ACS Omega, 2021, 6, 27898-27904.	3.5	2
126	Structural and electronic properties of zigzag InP nanoribbons with Stoneâ€“Wales type defects. Journal of Physics Condensed Matter, 2016, 28, 065503.	1.8	1

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127	Hydrodynamic signatures in thermal transport in devices based on two-dimensional materials: An ab initio study. Physical Review B, 2022, 106, .	3.2	1
128	The AFLOW Fleet for Materials Discovery. , 2019, , 1-28.		0