Jess Carrete

List of Publications by Citations

123 papers	5,747 citations	40 h-index	74 g-index
128 ext. papers	6,935 ext. citations	5 avg, IF	6.21 L-index

#	Paper	IF	Citations
123	ShengBTE: A solver of the Boltzmann transport equation for phonons. *Computer Physics Communications*, **2014**, 185, 1747-1758	4.2	1243
122	BoltzTraP2, a program for interpolating band structures and calculating semi-classical transport coefficients. *Computer Physics Communications*, **2018**, 231, 140-145	4.2	320
121	Phonon thermal transport in strained and unstrained graphene from first principles. *Physical Review B*, **2014**, 89,	3.3	270
120	Thermal conductivity and phonon linewidths of monolayer MoS2 from first principles. *Applied Physics Letters*, **2013**, 103, 253103	3.4	236
119	Low thermal conductivity and triaxial phononic anisotropy of SnSe. *Applied Physics Letters*, **2014**, 105, 101907	3.4	200
118	Finding Unprecedentedly Low-Thermal-Conductivity Half-Heusler Semiconductors via High-Throughput Materials Modeling. *Physical Review X*, **2014**, 4,	9.1	168
117	Physically founded phonon dispersions of few-layer materials and the case of borophene. *Materials Research Letters*, **2016**, 4, 204-211	7.4	158
116	almaBTE : A solver of the space□time dependent Boltzmann transport equation for phonons in structured materials. *Computer Physics Communications*, **2017**, 220, 351-362	4.2	124
115	Strong enhancement of phonon scattering through nanoscale grains in lead sulfide thermoelectrics. *NPG Asia Materials*, **2014**, 6, e108-e108	10.3	119
114	Molecular dynamics simulation of the structure and dynamics of water-1-alkyl-3-methylimidazolium ionic liquid mixtures. *Journal of Physical Chemistry B*, **2011**, 115, 6995-7008	3.4	111
113	Unexpected high-temperature stability of □Zn4Sb3 opens the door to enhanced thermoelectric performance. *Journal of the American Chemical Society*, **2014**, 136, 1497-504	16.4	97
112	Nanograined Half-Heusler Semiconductors as Advanced Thermoelectrics: An Ab Initio High-Throughput Statistical Study. *Advanced Functional Materials*, **2014**, 24, 7427-7432	15.6	97
111	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, 3207-20	3.4	77
110	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, 11302-12	3.4	77
109	Temperature and Thickness Dependences of the Anisotropic In-Plane Thermal Conductivity of Black Phosphorus. *Advanced Materials*, **2017**, 29, 1603756	24	75
108	Solvation of lithium salts in protic ionic liquids: a molecular dynamics study. *Journal of Physical Chemistry B*, **2014**, 118, 761-70	3.4	74
107	Effect of nitrogen and vacancy defects on the thermal conductivity of diamond: An ab initio Green□function approach. *Physical Review B*, **2014**, 90,	3.3	72

106	Solvation of molecular cosolvents and inorganic salts in ionic liquids: A review of molecular dynamics simulations. *Journal of Molecular Liquids*, **2015**, 210, 178-188	6	70
105	Surface roughness and thermal conductivity of semiconductor nanowires: Going below the Casimir limit. *Physical Review B*, **2011**, 84,	3.3	70
104	How Chemical Composition Alone Can Predict Vibrational Free Energies and Entropies of Solids. *Chemistry of Materials*, **2017**, 29, 6220-6227	9.6	69
103	Mixtures of protic ionic liquids and molecular cosolvents: a molecular dynamics simulation. *Journal of Chemical Physics*, **2014**, 140, 214502	3.9	69
102	Materials Screening for the Discovery of New Half-Heuslers: Machine Learning versus ab Initio Methods. *Journal of Physical Chemistry B*, **2018**, 122, 625-632	3.4	60
101	Superdiffusive heat conduction in semiconductor alloys. I. Theoretical foundations. *Physical Review B*, **2015**, 91,	3.3	59
100	Molecular dynamics simulations of the structure of the graphene-ionic liquid/alkali salt mixtures interface. *Physical Chemistry Chemical Physics*, **2014**, 16, 13271-8	3.6	54
99	Liquid□Solid□Liquid phase transition hysteresis loops in the ionic conductivity of ten imidazolium-based ionic liquids. *Fluid Phase Equilibria*, **2012**, 320, 1-10	2.5	54
98	Exceptionally Strong Phonon Scattering by B Substitution in Cubic SiC. *Physical Review Letters*, **2017**, 119, 075902	7.4	53
97	Ab initio study of the effect of vacancies on the thermal conductivity of boron arsenide. *Physical Review B*, **2016**, 94,	3.3	53
96	Twisting phonons in complex crystals with quasi-one-dimensional substructures. *Nature Communications*, **2015**, 6, 6723	17.4	52
95	Molecular dynamics simulations of the structural and thermodynamic properties of imidazolium-based ionic liquid mixtures. *Journal of Physical Chemistry B*, **2011**, 115, 11170-82	3.4	51
94	AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. *Computational Materials Science*, **2018**, 152, 134-145	3.2	51
93	How does lithium nitrate dissolve in a protic ionic liquid?. *Journal of Molecular Liquids*, **2015**, 205, 16-21	6	50
92	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	6.7	48
91	An efficient and accurate framework for calculating lattice thermal conductivity of solids: AFLOW□AAPL Automatic Anharmonic Phonon Library. *Npj Computational Materials*, **2017**, 3,	10.9	46
90	Ab initio study of 3d, 4d, and 5d transition metal adatoms and dimers adsorbed on hydrogen-passivated zigzag graphene nanoribbons. *Physical Review B*, **2011**, 83,	3.3	45
89	Anomalous pressure dependence of thermal conductivities of large mass ratio compounds. *Physical Review B*, **2015**, 91,	3.3	44

88	Ab initio phonon scattering by dislocations. *Physical Review B*, **2017**, 95,	3.3	43
87	Pseudolattice theory of charge transport in ionic solutions: Corresponding states law for the electric conductivity. *Fluid Phase Equilibria*, **2010**, 298, 280-286	2.5	43
86	Structural, magnetic, and electronic properties of Nin and Fen nanostructures (n=1–4) adsorbed on zigzag graphene nanoribbons. *Physical Review B*, **2010**, 81,	3.3	41
85	High-Throughput Computation of Thermal Conductivity of High-Temperature Solid Phases: The Case of Oxide and Fluoride Perovskites. *Physical Review X*, **2016**, 6,	9.1	41
84	Anomalous thermal conductivity and suppression of negative thermal expansion in ScF3. *Physical Review B*, **2016**, 94,	3.3	41
83	Surfactant self-assembly nanostructures in protic ionic liquids. *Journal of Physical Chemistry B*, **2011** , 115, 8145-54	3.4	40
82	Cross-plane heat conduction in thin films with ab-initio phonon dispersions and scattering rates. *Applied Physics Letters*, **2016**, 108, 193104	3.4	36
81	Unraveling the dominant phonon scattering mechanism in the thermoelectric compound ZrNiSn. *Journal of Materials Chemistry A*, **2016**, 4, 15940-15944	13	36
80	Structural Complexity and Phonon Physics in 2D Arsenenes. *Journal of Physical Chemistry Letters*, **2017**, 8, 1375-1380	6.4	34
79	Nanostructure of mixtures of protic ionic liquids and lithium salts: effect of alkyl chain length. *Physical Chemistry Chemical Physics*, **2015**, 17, 5298-307	3.6	34
78	Influence of the optical-acoustic phonon hybridization on phonon scattering and thermal conductivity. *Physical Review B*, **2016**, 93,	3.3	33
77	Dynamical properties of alcohol + 1-hexyl-3-methylimidazolium ionic liquid mixtures: a computer simulation study. *Journal of Physical Chemistry B*, **2011**, 115, 15313-22	3.4	31
76	Re-entrant phase behavior for systems with competition between phase separation and self-assembly. *Journal of Chemical Physics*, **2011**, 134, 104905	3.9	30
75	Phonon thermal transport in 2H, 4H and 6H silicon carbide from first principles. *Materials Today Physics*, **2017**, 1, 31-38	8	29
74	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	3.6	28
73	Pseudolattice theory of the surface tension of ionic liquid-water mixtures. *Journal of Physical Chemistry B*, **2009**, 113, 12500-5	3.4	27
72	Magnetism of substitutional Fe impurities in graphene nanoribbons. *Journal of Chemical Physics*, **2011**, 134, 024704	3.9	26
71	Al enhances the H2 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,	3.3	24

70	First-principles quantitative prediction of the lattice thermal conductivity in random semiconductor alloys: The role of force-constant disorder. *Physical Review B*, **2018**, 98,	3.3	24
69	Thermoelectric Properties of Hybrid Organic□Inorganic Superlattices. *Journal of Physical Chemistry C*, **2012**, 116, 10881-10886	3.8	23
68	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, 5941-50	3.4	22
67	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	3.8	21
66	Ultralow lattice thermal conductivity in topological insulator TlBiSe2. *Applied Physics Letters*, **2016**, 108, 233902	3.4	19
65	Thermal transport through Ge-rich Ge/Si superlattices grown on Ge(0 0 1). *Journal Physics D: Applied Physics*, **2018**, 51, 014001	3	19
64	Phonon Scattering by Dislocations in GaN. *ACS Applied Materials & Interfaces*, **2019**, 11, 8175-8181	9.5	18
63	Independently tuning the power factor and thermal conductivity of SnSe via Ag2S addition and nanostructuring. *Journal of Materials Chemistry A*, **2018**, 6, 7959-7966	13	17
62	Molecular hydrogen uptake by zigzag graphene nanoribbons doped with early 3d transition-metal atoms. *International Journal of Hydrogen Energy*, **2013**, 38, 8872-8880	6.7	17
61	Phonon transport unveils the prevalent point defects in GaN. *Physical Review Materials*, **2018**, 2,	3.2	17
60	Ultrahigh Thermal Conductivity of □Phase Tantalum Nitride. *Physical Review Letters*, **2021**, 126, 115901	7.4	16
59	Thermal Resistance of GaN/AlN Graded Interfaces. *Physical Review Applied*, **2019**, 11,	4.3	15
58	Influence of point defects on the thermal conductivity in FeSi. *Physical Review B*, **2018**, 97,	3.3	15
57	Microstructure investigations and thermoelectrical properties of an N-type magnesium□silicon□tin alloy sintered from a gas-phase atomized powder. *Acta Materialia*, **2015**, 96, 437-451	8.4	14
56	Atomistic origin of glass-like Zn4Sb3 thermal conductivity. *Applied Physics Letters*, **2013**, 103, 103902	3.4	14
55	Thermal Conductivity of Ionic Liquids: A Pseudolattice Approach. *Journal of Physical Chemistry C*, **2012**, 116, 1265-1273	3.8	14
54	Resonant phonon scattering in semiconductors. *Journal of Materials Chemistry C*, **2018**, 6, 4691-4697	7.1	13
53	Influence of Antisite Defects on the Thermoelectric Properties of Fe2VAl. *Nanoscale and Microscale Thermophysical Engineering*, **2017**, 21, 237-246	3.7	13

52	Theoretical model for moisture adsorption on ionic liquids: A modified Brunauer–Emmett–Teller isotherm approach. *Fluid Phase Equilibria*, **2011**, 301, 118-122	2.5	13
51	Nonextensive statistical mechanics of ionic solutions. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2007**, 370, 405-412	2.3	13
50	Human Immune Protein C1q Selectively Disaggregates Carbon Nanotubes. *Nano Letters*, **2017**, 17, 3409-3415	11.5	12
49	Predictive Design and Experimental Realization of InAs/GaAs Superlattices with Tailored Thermal Conductivity. *Journal of Physical Chemistry C*, **2018**, 122, 4054-4062	3.8	12
48	Role of force-constant difference in phonon scattering by nano-precipitates in PbTe. *Journal of Applied Physics*, **2015**, 118, 085701	2.5	12
47	Molecular-dynamics prediction of the thermal conductivity of thin InP nanowires: Similarities to Si. *Physical Review B*, **2009**, 80,	3.3	12
46	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	13	12
45	A theoretical model of the thermoelectric properties of SnSxSe1−x and how to further enhance its thermoelectric performance. *Journal of Applied Physics*, **2019**, 126, 225105	2.5	12
44	Anomalously large lattice thermal conductivity in metallic tungsten carbide and its origin in the electronic structure. *Materials Today Physics*, **2020**, 13, 100214	8	11
43	Ab initio lattice thermal conductivity of bulk and thin-film α-Al2O3. *MRS Communications*, **2018**, 8, 1119-1123	2.3	10
42	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	3.4	10
41	Shortcomings of meta-GGA functionals when describing magnetism. *Physical Review B*, **2020**, 102,	3.3	9
40	The Effect of Janus Asymmetry on Thermal Transport in SnSSe. *Journal of Physical Chemistry C*, **2020**, 124, 17476-17484	3.8	9
39	Basal-plane thermal conductivity of nanocrystalline and amorphized thin germanane. *Applied Physics Letters*, **2016**, 109, 131907	3.4	9
38	The AFLOW Fleet for Materials Discovery **2018**, 1-28		9
37	Density Functional Study of Charge Transfer at the Graphene/Ionic Liquid Interface. *Journal of Physical Chemistry C*, **2018**, 122, 15070-15077	3.8	9
36	Phonon transport across crystal-phase interfaces and twin boundaries in semiconducting nanowires. *Nanoscale*, **2019**, 11, 16007-16016	7.7	7
35	A density-functional study of the structures and electronic properties of neutral, anionic, and endohedrally doped In(x)P(x) clusters. *Journal of Chemical Physics*, **2009**, 131, 074504	3.9	7

34	Complex Network Analysis in Socioeconomic Models. *Dynamic Modeling and Econometrics in Economics and Finance*, **2015**, 209-245		7
33	Borophene vs. graphene interfaces: Tuning the electric double layer in ionic liquids. *Journal of Molecular Liquids*, **2020**, 303, 112647	6	7
32	Vibrational Properties of Metastable Polymorph Structures by Machine Learning. *Journal of Chemical Information and Modeling*, **2018**, 58, 2460-2466	6.1	7
31	Machine-learning Prediction of Infrared Spectra of Interstellar Polycyclic Aromatic Hydrocarbons. *Astrophysical Journal*, **2020**, 902, 100	4.7	6
30	Optimisation of the thermoelectric efficiency of zirconium trisulphide monolayers through unixial and biaxial strain. *Nanoscale Advances*, **2020**, 2, 5352-5361	5.1	6
29	Influence of the addition of Half-Heusler nanoparticles on the thermoelectrical properties of an N-type magnesium□silicon□tin alloy. *Scripta Materialia*, **2015**, 104, 5-8	5.6	5
28	Anisotropic Thermal Conductivity in Few-Layer and Bulk Titanium Trisulphide from First Principles. *Nanomaterials*, **2020**, 10,	5.4	5
27	Glass-like thermal conductivity in nanostructures of a complex anisotropic crystal. *Physical Review B* , **2017**, 96,	3.3	5
26	A density-functional study of the vertical ionization potentials of the cluster Mn13. *Journal of Chemical Physics*, **2009**, 131, 046101	3.9	5
25	Nonequilibrium nanothermodynamics. *Physical Review E*, **2008**, 77, 022102	2.4	5
24	Effect of local chemistry and structure on thermal transport in doped GaAs. *Physical Review Materials*, **2019**, 3,	3.2	5
23	How dopants limit the ultrahigh thermal conductivity of boron arsenide: a first principles study. *Npj Computational Materials*, **2021**, 7,	10.9	5
22	Understanding Phonon Scattering by Nanoprecipitates in Potassium-Doped Lead Chalcogenides. *ACS Applied Materials & Interfaces*, **2017**, 9, 3686-3693	9.5	4
21	Coupling of Spinons with Defects and Phonons in the Spin Chain Compound Ca_{2}CuO_{3}. *Physical Review Letters*, **2019**, 122, 185901	7.4	4
20	Growth, charge and thermal transport of flowered graphene. *Carbon*, **2020**, 161, 259-268	10.4	4
19	Optimizing phonon scattering by nanoprecipitates in lead chalcogenides. *Applied Physics Letters*, **2016**, 108, 113901	3.4	4
18	Microcanonical equations obtained from the Tsallis entropy. *Physica A: Statistical Mechanics and Its Applications*, **2008**, 387, 6752-6758	3.3	4
17	Localized dimers drive strong anharmonicity and low lattice thermal conductivity in ZnSe2. *Physical Review B*, **2020**, 102,	3.3	4

16	Parameter-free model to estimate thermal conductivity in nanostructured materials. *Physical Review B*, **2019**, 100,	3.3	3
15	High-throughput study of the static dielectric constant at high temperatures in oxide and fluoride cubic perovskites. *Physical Review Materials*, **2020**, 4,	3.2	3
14	Tunable gap in stable arsenene nanoribbons opens the door to electronic applications.. *RSC Advances*, **2019**, 9, 11818-11823	3.7	2
13	Using nanotubes to study the phonon spectrum of two-dimensional materials. *Physical Chemistry Chemical Physics*, **2019**, 21, 5215-5223	3.6	2
12	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	2
11	Structural, magnetic, and vibrational properties of stoichiometric clusters of CrN. *International Journal of Quantum Chemistry*, **2015**, 115, 523-528	2.1	2
10	Twisted bilayer graphene as a linear nanoactuator. *Physical Review B*, **2020**, 102,	3.3	2
9	Pseudolattice Theory of Ionic Liquids **2011**,		1
8	Influence of Onion-like Carbonaceous Particles on the Aggregation Process of Hydrocarbons. *ACS Omega*, **2021**, 6, 27898-27904	3.9	1
7	The AFLOW Fleet for Materials Discovery **2020**, 1785-1812		1
6	Effects of doping substitutions on the thermal conductivity of half-Heusler compounds. *Physical Review B*, **2021**, 103,	3.3	1
5	Quantum Self-Consistent Ab-Initio Lattice Dynamics. *Computer Physics Communications*, **2021**, 263, 107945	4.2	1
4	Thermoelectric properties of the SnS monolayer: Fully ab initio and accelerated calculations. *Journal of Applied Physics*, **2021**, 130, 054301	2.5	1
3	Strain-tunable lattice thermal conductivity of the Janus PtSTe monolayer. *Journal of Physics Condensed Matter*, **2021**, 34,	1.8	1
2	Structural and electronic properties of zigzag InP nanoribbons with Stone-Wales type defects. *Journal of Physics Condensed Matter*, **2016**, 28, 065503	1.8	0
1	The AFLOW Fleet for Materials Discovery **2019**, 1-28		