# JesÃºs Carrete

List of Publications by Year
in descending order

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Version: 2024-02-01

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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 | Strain-tunable lattice thermal conductivity of the Janus PtSTe monolayer. Journal of Physics Condensed Matter, 2022, 34, 015303. | 1.8 | 6 |
| 2 | A Differentiable Neural-Network Force Field for Ionic Liquids. Journal of Chemical Information and Modeling, 2022, 62, 88-101. | 5.4 | 17 |
| 3 | 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></ Physical Review B, 2022, 105, . | 3.2 | 6 |
| 4 | Hydrodynamic signatures in thermal transport in devices based on two-dimensional materials: An ab initio study. Physical Review B, 2022, 106, . | 3.2 | 1 |
| 5 | 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 |
| 6 | How dopants limit the ultrahigh thermal conductivity of boron arsenide: a first principles study. Npj Computational Materials, 2021, 7, . | 8.7 | 21 |
| 7 | 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 |
| 8 | Effects of doping substitutions on the thermal conductivity of half-Heusler compounds. Physical Review B, 2021, 103, . | 3.2 | 5 |
| 9 | Quantum Self-Consistent Ab-Initio Lattice Dynamics. Computer Physics Communications, 2021, 263, 107945. | 7.5 | 18 |
| 10 | Thermoelectric properties of the SnS monolayer: Fully ab initio and accelerated calculations. Journal of Applied Physics, 2021, 130, . | 2.5 | 15 |
| 11 | Influence of Onion-like Carbonaceous Particles on the Aggregation Process of Hydrocarbons. ACS Omega, 2021, 6, 27898-27904. | 3.5 | 2 |
| 12 | 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 |
| 13 | 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:mn Physical Review B, 2020, 102, . | 3.2 | 17 |
| 14 | Shortcomings of meta-GGA functionals when describing magnetism. Physical Review B, 2020, 102, . | 3.2 | 27 |
| 15 | The Effect of Janus Asymmetry on Thermal Transport in SnSSe. Journal of Physical Chemistry C, 2020, 124, 17476-17484. | 3.1 | 30 |
| 16 | Borophene vs. graphene interfaces: Tuning the electric double layer in ionic liquids. Journal of Molecular Liquids, 2020, 303, 112647. | 4.9 | 8 |
| 17 | Twisted bilayer graphene as a linear nanoactuator. Physical Review B, 2020, 102, . | 3.2 | 4 |
| 18 | Growth, charge and thermal transport of flowered graphene. Carbon, 2020, 161, 259-268. | 10.3 | 7 |

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| 19 | Anisotropic Thermal Conductivity in Few-Layer and Bulk Titanium Trisulphide from First Principles. Nanomaterials, 2020, 10, 704. | 4.1 | 8 |
| 20 | 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 |
| 21 | Optimisation of the thermoelectric efficiency of zirconium trisulphide monolayers through unixial and biaxial strain. Nanoscale Advances, 2020, 2, 5352-5361. | 4.6 | 8 |
| 22 | 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 |
| 23 | Machine-learning Prediction of Infrared Spectra of Interstellar Polycyclic Aromatic Hydrocarbons. Astrophysical Journal, 2020, 902, 100. | 4.5 | 16 |
| 24 | The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812. | | 4 |
| 25 | Phonon transport across crystal-phase interfaces and twin boundaries in semiconducting nanowires. Nanoscale, 2019, 11, 16007-16016. | 5.6 | 17 |
| 26 | Parameter-free model to estimate thermal conductivity in nanostructured materials. Physical Review B, 2019, 100, . | 3.2 | 11 |
| 27 | Phonon Scattering by Dislocations in GaN. ACS Applied Materials & Interfaces, 2019, 11, 8175-8181. | 8.0 | 25 |
| 28 | 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><mm Physical Review Letters, 2019, 122, 185901. | 7.8 | 9 |
| 29 | Tunable gap in stable arsenene nanoribbons opens the door to electronic applications. RSC Advances, 2019, 9, 11818-11823. | 3.6 | 3 |
| 30 | The AFLOW Fleet for Materials Discovery. , 2019, , 1-28. | | 0 |
| 31 | 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 Appli | 3.8 | 17 |
| 32 | Using nanotubes to study the phonon spectrum of two-dimensional materials. Physical Chemistry Chemical Physics, 2019, 21, 5215-5223. | 2.8 | 3 |
| 33 | 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 |
| 34 | Effect of local chemistry and structure on thermal transport in doped GaAs. Physical Review Materials, 2019, 3, . | 2.4 | 9 |
| 35 | 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 |
| 36 | Resonant phonon scattering in semiconductors. Journal of Materials Chemistry C, 2018, 6, 4691-4697. | 5.5 | 17 |

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| 37 | 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 |
| 38 | 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 |
| 39 | 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 |
| 40 | 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 |
| 41 | The AFLOW Fleet for Materials Discovery. , 2018, , 1-28. | | 9 |
| 42 | 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 |
| 43 | Vibrational Properties of Metastable Polymorph Structures by Machine Learning. Journal of Chemical Information and Modeling, 2018, 58, 2460-2466. | 5.4 | 14 |
| 44 | BoltzTraP2, a program for interpolating band structures and calculating semi-classical transport coefficients. Computer Physics Communications, 2018, 231, 140-145. | 7.5 | 730 |
| 45 | AFLOW-ML: A RESTful API for machine-learning predictions of materials properties. Computational Materials Science, 2018, 152, 134-145. | 3.0 | 72 |
| 46 | Density Functional Study of Charge Transfer at the Graphene/Ionic Liquid Interface. Journal of Physical Chemistry C, 2018, 122, 15070-15077. | 3.1 | 11 |
| 47 | Influence of point defects on the thermal conductivity in FeSi. Physical Review B, 2018, 97, . | 3.2 | 21 |
| 48 | Ab initio lattice thermal conductivity of bulk and thin-film Î±-Al2O3. MRS Communications, 2018, 8, 1119-1123. | 1.8 | 17 |
| 49 | Phonon transport unveils the prevalent point defects in GaN. Physical Review Materials, 2018, 2, . | 2.4 | 22 |
| 50 | Understanding Phonon Scattering by Nanoprecipitates in Potassium-Doped Lead Chalcogenides. ACS Applied Materials & Interfaces, 2017, 9, 3686-3693. | 8.0 | 6 |
| 51 | How Chemical Composition Alone Can Predict Vibrational Free Energies and Entropies of Solids. Chemistry of Materials, 2017, 29, 6220-6227. | 6.7 | 103 |
| 52 | Human Immune Protein C1q Selectively Disaggregates Carbon Nanotubes. Nano Letters, 2017, 17, 3409-3415. | 9.1 | 14 |
| 53 | Structural Complexity and Phonon Physics in 2D Arsenenes. Journal of Physical Chemistry Letters, 2017, 8, 1375-1380. | 4.6 | 41 |
| 54 | 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 |

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| 55 | 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 |
| 56 | Exceptionally Strong Phonon Scattering by B Substitution in Cubic SiC. Physical Review Letters, 2017, 119, 075902. | 7.8 | 68 |
| 57 | Influence of Antisite Defects on the Thermoelectric Properties of Fe<sub>2</sub>VAl. Nanoscale and Microscale Thermophysical Engineering, 2017, 21, 237-246. | 2.6 | 16 |
| 58 | Phonon thermal transport in 2H, 4H and 6H silicon carbide from first principles. Materials Today Physics, 2017, 1, 31-38. | 6.0 | 48 |
| 59 | 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 |
| 60 | Ab initio phonon scattering by dislocations. Physical Review B, 2017, 95, . | 3.2 | 49 |
| 61 | Temperature and Thickness Dependences of the Anisotropic Inâ€Plane Thermal Conductivity of Black Phosphorus. Advanced Materials, 2017, 29, 1603756. | 21.0 | 99 |
| 62 | Glass-like thermal conductivity in nanostructures of a complex anisotropic crystal. Physical Review B, 2017, 96, . | 3.2 | 10 |
| 63 | Physically founded phonon dispersions of few-layer materials and the case of borophene. Materials Research Letters, 2016, 4, 204-211. | 8.7 | 216 |
| 64 | Cross-plane heat conduction in thin films with ab-initio phonon dispersions and scattering rates. Applied Physics Letters, 2016, 108, . | 3.3 | 44 |
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| 66 | Unraveling the dominant phonon scattering mechanism in the thermoelectric compound ZrNiSn. Journal of Materials Chemistry A, 2016, 4, 15940-15944. | 10.3 | 40 |
| 67 | Ultralow lattice thermal conductivity in topological insulator TlBiSe2. Applied Physics Letters, 2016, 108, . | 3.3 | 29 |
| 68 | Basal-plane thermal conductivity of nanocrystalline and amorphized thin germanane. Applied Physics Letters, 2016, 109, 131907. | 3.3 | 11 |
| 69 | 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 | 51 |
| 70 | Ab initiostudy of the effect of vacancies on the thermal conductivity of boron arsenide. Physical Review B, 2016, 94, . | 3.2 | 65 |
| 71 | 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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| 74 | Anomalous pressure dependence of thermal conductivities of large mass ratio compounds. Physical Review B, 2015, 91, . | 3.2 | 71 |
| 75 | Role of force-constant difference in phonon scattering by nano-precipitates in PbTe. Journal of Applied Physics, 2015, 118, . | 2.5 | 12 |
| 76 | 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 |
| 77 | How does lithium nitrate dissolve in a protic ionic liquid?. Journal of Molecular Liquids, 2015, 205, 16-21. | 4.9 | 53 |
| 78 | Superdiffusive heat conduction in semiconductor alloys. I. Theoretical foundations. Physical Review B, 2015, 91, . | 3.2 | 75 |
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| 82 | Twisting phonons in complex crystals with quasi-one-dimensional substructures. Nature Communications, 2015, 6, 6723. | 12.8 | 75 |
| 83 | 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 |
| 84 | 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 |
| 85 | Complex Network Analysis in Socioeconomic Models. Dynamic Modeling and Econometrics in Economics and Finance, 2015, , 209-245. | 0.5 | 13 |
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| 88 | Finding Unprecedentedly Low-Thermal-Conductivity Half-Heusler Semiconductors via High-Throughput Materials Modeling. Physical Review X, 2014, 4, . | 8.9 | 210 |
| 89 | Solvation of Lithium Salts in Protic Ionic Liquids: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2014, 118, 761-770. | 2.6 | 87 |
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| 93 | 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 |
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| 98 | 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 |
| 99 | Thermal conductivity and phonon linewidths of monolayer MoS2 from first principles. Applied Physics Letters, 2013, 103, . | 3.3 | 273 |
| 100 | Atomistic origin of glass-like Zn4Sb3 thermal conductivity. Applied Physics Letters, 2013, 103, 103902. | 3.3 | 15 |
| 101 | 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 |
| 102 | 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 |
| 103 | Thermal Conductivity of Ionic Liquids: A Pseudolattice Approach. Journal of Physical Chemistry C, 2012, 116, 1265-1273. | 3.1 | 18 |
| 104 | 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 |
| 105 | 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 |
| 106 | Thermoelectric Properties of Hybrid Organicâ€“Inorganic Superlattices. Journal of Physical Chemistry C, 2012, 116, 10881-10886. | 3.1 | 24 |
| 107 | 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 |
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| 109 | Surfactant Self-Assembly Nanostructures in Protic Ionic Liquids. Journal of Physical Chemistry B, 2011, 115, 8145-8154. | 2.6 | 47 |
| 110 | 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 |
| 111 | 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 |
| 112 | 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 |
| 113 | Magnetism of substitutional Fe impurities in graphene nanoribbons. Journal of Chemical Physics, 2011, 134, 024704. | 3.0 | 29 |
| 114 | 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 |
| 115 | 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 |
| 116 | Pseudolattice Theory of Ionic Liquids. , 2011, , . | | 2 |
| 117 | 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 |
| 118 | Surface roughness and thermal conductivity of semiconductor nanowires: Going below the Casimir limit. Physical Review B, 2011, 84, . | 3.2 | 74 |
| 119 | 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 |
| 120 | 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 |
| 121 | A density-functional study of the vertical ionization potentials of the cluster Mn13. Journal of Chemical Physics, 2009, 131, 046101. | 3.0 | 5 |
| 122 | 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 |
| 123 | Pseudolattice Theory of the Surface Tension of Ionic Liquidâ^'Water Mixtures. Journal of Physical Chemistry B, 2009, 113, 12500-12505. | 2.6 | 30 |
| 124 | Molecular-dynamics prediction of the thermal conductivity of thin InP nanowires: Similarities to Si. Physical Review B, 2009, 80, . | 3.2 | 12 |
| 125 | Microcanonical equations obtained from the Tsallis entropy. Physica A: Statistical Mechanics and Its Applications, 2008, 387, 6752-6758. | 2.6 | 4 |
| 126 | Nonequilibrium nanothermodynamics. Physical Review E, 2008, 77, 022102. | 2.1 | 6 |

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