# Feliciano Giustino

## List of Publications by Citations



| | | | |
|---|---|---|---|
| 164 papers | 15,554 citations | 54 h-index | 124 g-index |
| 179 ext. papers | 19,264 ext. citations | 7.5 avg, IF | 7.33 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 164 | Advanced capabilities for materials modelling with Quantum ESPRESSO. *Journal of Physics Condensed Matter*, **2017**, 29, 465901 | 1.8 | 2275 |
| 163 | Perovskite-perovskite tandem photovoltaics with optimized band gaps. *Science*, **2016**, 354, 861-865 | 33.3 | 865 |
| 162 | Electron-phonon coupling in hybrid lead halide perovskites. *Nature Communications*, **2016**, 7, | 17.4 | 668 |
| 161 | Toward Lead-Free Perovskite Solar Cells. *ACS Energy Letters*, **2016**, 1, 1233-1240 | 20.1 | 636 |
| 160 | Steric engineering of metal-halide perovskites with tunable optical band gaps. *Nature Communications*, **2014**, 5, 5757 | 17.4 | 605 |
| 159 | Lead-Free Halide Double Perovskites via Heterovalent Substitution of Noble Metals. *Journal of Physical Chemistry Letters*, **2016**, 7, 1254-9 | 6.4 | 567 |
| 158 | Electron-phonon interactions from first principles. *Reviews of Modern Physics*, **2017**, 89, | 40.5 | 538 |
| 157 | CsInAgCl: A New Lead-Free Halide Double Perovskite with Direct Band Gap. *Journal of Physical Chemistry Letters*, **2017**, 8, 772-778 | 6.4 | 494 |
| 156 | EPW: Electron□phonon coupling, transport and superconducting properties using maximally localized Wannier functions. *Computer Physics Communications*, **2016**, 209, 116-133 | 4.2 | 433 |
| 155 | Electron-phonon interaction using Wannier functions. *Physical Review B*, **2007**, 76, | 3.3 | 425 |
| 154 | Band Gaps of the Lead-Free Halide Double Perovskites Cs2BiAgCl6 and Cs2BiAgBr6 from Theory and Experiment. *Journal of Physical Chemistry Letters*, **2016**, 7, 2579-85 | 6.4 | 395 |
| 153 | TiO2 anatase with a bandgap in the visible region. *Nano Letters*, **2014**, 14, 6533-8 | 11.5 | 384 |
| 152 | Dislocation-driven deformations in graphene. *Science*, **2012**, 337, 209-12 | 33.3 | 295 |
| 151 | Cubic or Orthorhombic? Revealing the Crystal Structure of Metastable Black-Phase CsPbI3 by Theory and Experiment. *ACS Energy Letters*, **2018**, 3, 1787-1794 | 20.1 | 292 |
| 150 | Oxygen redox chemistry without excess alkali-metal ions in Na[MgMn]O. *Nature Chemistry*, **2018**, 10, 288-295 | 17.6 | 281 |
| 149 | EPW: A program for calculating the electron□phonon coupling using maximally localized Wannier functions. *Computer Physics Communications*, **2010**, 181, 2140-2148 | 4.2 | 225 |
| 148 | Vibrational Properties of the Organic□Inorganic Halide Perovskite CH3NH3PbI3 from Theory and Experiment: Factor Group Analysis, First-Principles Calculations, and Low-Temperature Infrared Spectra. *Journal of Physical Chemistry C*, **2015**, 119, 25703-25718 | 3.8 | 220 |

| | | | |
|---|---|---|---|
| 147 | Confinement Effects in Low-Dimensional Lead Iodide Perovskite Hybrids. *Chemistry of Materials*, **2016**, 28, 4554-4562 | 9.6 | 203 |
| 146 | Electron-phonon renormalization of the direct band gap of diamond. *Physical Review Letters*, **2010**, 105, 265501 | 7.4 | 192 |
| 145 | Bimolecular recombination in methylammonium lead triiodide perovskite is an inverse absorption process. *Nature Communications*, **2018**, 9, 293 | 17.4 | 175 |
| 144 | Fröhlich Electron-Phonon Vertex from First Principles. *Physical Review Letters*, **2015**, 115, 176401 | 7.4 | 165 |
| 143 | Computational Screening of Homovalent Lead Substitution in Organic–Inorganic Halide Perovskites. *Journal of Physical Chemistry C*, **2016**, 120, 166-173 | 3.8 | 162 |
| 142 | Velocity renormalization and carrier lifetime in graphene from the electron-phonon interaction. *Physical Review Letters*, **2007**, 99, 086804 | 7.4 | 162 |
| 141 | GW quasiparticle band structures of stibnite, antimonselite, bismuthinite, and guanajuatite. *Physical Review B*, **2013**, 87, | 3.3 | 142 |
| 140 | Band offsets at the Si/SiO2 interface from many-body perturbation theory. *Physical Review Letters*, **2008**, 100, 186401 | 7.4 | 141 |
| 139 | First-principles prediction of doped graphane as a high-temperature electron-phonon superconductor. *Physical Review Letters*, **2010**, 105, 037002 | 7.4 | 140 |
| 138 | Electron-phonon interactions in graphene, bilayer graphene, and graphite. *Nano Letters*, **2008**, 8, 4229-33 | 11.5 | 138 |
| 137 | Small phonon contribution to the photoemission kink in the copper oxide superconductors. *Nature*, **2008**, 452, 975-8 | 50.4 | 135 |
| 136 | Solution-Processed Cesium Hexabromopalladate(IV), CsPdBr, for Optoelectronic Applications. *Journal of the American Chemical Society*, **2017**, 139, 6030-6033 | 16.4 | 134 |
| 135 | Towards predictive many-body calculations of phonon-limited carrier mobilities in semiconductors. *Physical Review B*, **2018**, 97, | 3.3 | 128 |
| 134 | Anisotropic Migdal-Eliashberg theory using Wannier functions. *Physical Review B*, **2013**, 87, | 3.3 | 124 |
| 133 | Electron-phonon interaction via electronic and lattice Wannier functions: superconductivity in boron-doped diamond reexamined. *Physical Review Letters*, **2007**, 98, 047005 | 7.4 | 122 |
| 132 | GW Band Structures and Carrier Effective Masses of CH3NH3PbI3 and Hypothetical Perovskites of the Type APbI3: A = NH4, PH4, AsH4, and SbH4. *Journal of Physical Chemistry C*, **2015**, 119, 25209-25219 | 3.8 | 113 |
| 131 | Structural and Electronic Properties of Semiconductor-Sensitized Solar-Cell Interfaces. *Advanced Functional Materials*, **2011**, 21, 4663-4667 | 15.6 | 110 |
| 130 | Theory of atomic-scale dielectric permittivity at insulator interfaces. *Physical Review B*, **2005**, 71, | 3.3 | 108 |

| | | | |
|---|---|---|---|
| 129 | GW quasiparticle band gap of the hybrid organic-inorganic perovskite CH3NH3PbI3: Effect of spin-orbit interaction, semicore electrons, and self-consistency. *Physical Review B*, **2014**, 90, | 3.3 | 101 |
| 128 | GW method with the self-consistent Sternheimer equation. *Physical Review B*, **2010**, 81, | 3.3 | 98 |
| 127 | Angle-resolved photoemission spectra of graphene from first-principles calculations. *Nano Letters*, **2009**, 9, 4234-9 | 11.5 | 93 |
| 126 | Phase Diagrams and Stability of Lead-Free Halide Double Perovskites Cs2BB?X6: B = Sb and Bi, B? = Cu, Ag, and Au, and X = Cl, Br, and I. *Journal of Physical Chemistry C*, **2018**, 122, 158-170 | 3.8 | 91 |
| 125 | Origin of the crossover from polarons to Fermi liquids in transition metal oxides. *Nature Communications*, **2017**, 8, 15769 | 17.4 | 79 |
| 124 | Origin of Low Carrier Mobilities in Halide Perovskites. *ACS Energy Letters*, **2019**, 4, 456-463 | 20.1 | 79 |
| 123 | One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization. *Physical Review B*, **2016**, 94, | 3.3 | 77 |
| 122 | Quantum nuclear dynamics in the photophysics of diamondoids. *Nature Communications*, **2013**, 4, 2006 | 17.4 | 76 |
| 121 | Route to Stable Lead-Free Double Perovskites with the Electronic Structure of CHNHPbI: A Case for Mixed-Cation [Cs/CHNH/CH(NH)]InBiBr. *Journal of Physical Chemistry Letters*, **2017**, 8, 3917-3924 | 6.4 | 71 |
| 120 | Dielectric discontinuity at interfaces in the atomic-scale limit: permittivity of ultrathin oxide films on silicon. *Physical Review Letters*, **2003**, 91, 267601 | 7.4 | 71 |
| 119 | First-principles calculations of charge carrier mobility and conductivity in bulk semiconductors and two-dimensional materials. *Reports on Progress in Physics*, **2020**, 83, 036501 | 14.4 | 71 |
| 118 | The geometric blueprint of perovskites. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 5397-5402 | 11.5 | 70 |
| 117 | Origin of Superconductivity and Latent Charge Density Wave in NbS_{2}. *Physical Review Letters*, **2017**, 119, 087003 | 7.4 | 66 |
| 116 | First-principles study of electron linewidths in graphene. *Physical Review Letters*, **2009**, 102, 076803 | 7.4 | 65 |
| 115 | Stochastic Approach to Phonon-Assisted Optical Absorption. *Physical Review Letters*, **2015**, 115, 177401 | 7.4 | 63 |
| 114 | Graphene-based technologies for energy applications, challenges and perspectives. *2D Materials*, **2015**, 2, 030204 | 5.9 | 62 |
| 113 | Ferroelectric Graphene-Perovskite Interfaces. *Journal of Physical Chemistry Letters*, **2015**, 6, 2496-502 | 6.4 | 60 |
| 112 | Atomic-scale observation of multiconformational binding and energy level alignment of ruthenium-based photosensitizers on TiO2 anatase. *Nano Letters*, **2014**, 14, 563-9 | 11.5 | 60 |

| | | | |
|---|---|---|---|
| 111 | Structural and electronic properties of an abrupt 4H‐SiC(0001)/SiO2 interface model: Classical molecular dynamics simulations and density functional calculations. *Physical Review B*, **2007**, 76, | 3.3 | 55 |
| 110 | Ideal Energy-Level Alignment at the ZnO/P3HT Photovoltaic Interface. *Advanced Functional Materials*, **2012**, 22, 5089-5095 | 15.6 | 53 |
| 109 | Raman Spectrum of the Organic–Inorganic Halide Perovskite CH3NH3PbI3 from First Principles and High-Resolution Low-Temperature Raman Measurements. *Journal of Physical Chemistry C*, **2018**, 122, 21703-21717 | 3.8 | 53 |
| 108 | Strong carrier lifetime enhancement in GaAs nanowires coated with semiconducting polymer. *Nano Letters*, **2012**, 12, 6293-301 | 11.5 | 52 |
| 107 | GW quasiparticle bandgaps of anatase TiO2 starting from DFT + U. *Journal of Physics Condensed Matter*, **2012**, 24, 202201 | 1.8 | 52 |
| 106 | Two-gap superconductivity in heavily n-doped graphene: Ab initio Migdal-Eliashberg theory. *Physical Review B*, **2014**, 90, | 3.3 | 51 |
| 105 | Band structures of plasmonic polarons. *Physical Review Letters*, **2015**, 114, 146404 | 7.4 | 50 |
| 104 | Electron-phonon interaction and pairing mechanism in superconducting Ca-intercalated bilayer graphene. *Scientific Reports*, **2016**, 6, 21414 | 4.9 | 49 |
| 103 | Carrier Lifetimes and Polaronic Mass Enhancement in the Hybrid Halide Perovskite CH_{3}NH_{3}PbI_{3} from Multiphonon Fröhlich Coupling. *Physical Review Letters*, **2018**, 121, 086402 | 7.4 | 48 |
| 102 | Infrared spectra at surfaces and interfaces from first principles: evolution of the spectra across the Si(100)-SiO2 interface. *Physical Review Letters*, **2005**, 95, 187402 | 7.4 | 48 |
| 101 | The 2021 quantum materials roadmap. *JPhys Materials*, **2020**, 3, 042006 | 4.2 | 48 |
| 100 | Van Hove singularity and apparent anisotropy in the electron-phonon interaction in graphene. *Physical Review B*, **2008**, 77, | 3.3 | 46 |
| 99 | Unified theory of electron-phonon renormalization and phonon-assisted optical absorption. *Journal of Physics Condensed Matter*, **2014**, 26, 365503 | 1.8 | 42 |
| 98 | Atomistic models of the Si(100)/SiO2interface: structural, electronic and dielectric properties. *Journal of Physics Condensed Matter*, **2005**, 17, S2065-S2074 | 1.8 | 41 |
| 97 | Ultrafast entangling gates between nuclear spins using photoexcited triplet states. *Nature Physics*, **2012**, 8, 596-600 | 16.2 | 39 |
| 96 | Hole mobility of strained GaN from first principles. *Physical Review B*, **2019**, 100, | 3.3 | 38 |
| 95 | Electronic and dielectric properties of a suboxide interlayer at the silicon–oxide interface in MOS devices. *Surface Science*, **2005**, 586, 183-191 | 1.8 | 38 |
| 94 | Ab initio Sternheimer-GW method for quasiparticle calculations using plane waves. *Physical Review B*, **2013**, 88, | 3.3 | 35 |

| | | | |
|---|---|---|---|
| 93 | Dimensional Crossover in the Carrier Mobility of Two-Dimensional Semiconductors: The Case of InSe. *Nano Letters*, **2019**, 19, 1774-1781 | 11.5 | 34 |
| 92 | Surface properties of lead-free halide double perovskites: Possible visible-light photo-catalysts for water splitting. *Applied Physics Letters*, **2018**, 112, 243901 | 3.4 | 34 |
| 91 | Structure of a Water Monolayer on the Anatase TiO2(101) Surface. *Physical Review Applied*, **2014**, 2, | 4.3 | 34 |
| 90 | Ab initio theory of polarons: Formalism and applications. *Physical Review B*, **2019**, 99, | 3.3 | 32 |
| 89 | Polarons from First Principles, without Supercells. *Physical Review Letters*, **2019**, 122, 246403 | 7.4 | 32 |
| 88 | CaBaCo4O7: A ferrimagnetic pyroelectric. *Physical Review B*, **2014**, 90, | 3.3 | 32 |
| 87 | Route to High Hole Mobility in GaN via Reversal of Crystal-Field Splitting. *Physical Review Letters*, **2019**, 123, 096602 | 7.4 | 31 |
| 86 | Theory of electron-plasmon coupling in semiconductors. *Physical Review B*, **2016**, 94, | 3.3 | 29 |
| 85 | On the combined use of GW approximation and cumulant expansion in the calculations of quasiparticle spectra: The paradigm of Si valence bands. *Physical Review B*, **2016**, 94, | 3.3 | 28 |
| 84 | Origin of superconductivity in boron-doped silicon carbide from first principles. *Physical Review B*, **2009**, 79, | 3.3 | 26 |
| 83 | Nonadiabatic Kohn Anomaly in Heavily Boron-Doped Diamond. *Physical Review Letters*, **2017**, 119, 017001 | 7.4 | 25 |
| 82 | Quantitative analysis of valence photoemission spectra and quasiparticle excitations at chromophore-semiconductor interfaces. *Physical Review Letters*, **2012**, 109, 116801 | 7.4 | 24 |
| 81 | First-principles study of superconductivity and Fermi-surface nesting in ultrahard transition metal carbides. *Physical Review B*, **2008**, 77, | 3.3 | 24 |
| 80 | Dielectric effect of a thin SiO2 interlayer at the interface between silicon and high-k oxides. *Microelectronic Engineering*, **2004**, 72, 299-303 | 2.5 | 24 |
| 79 | Theory of the special displacement method for electronic structure calculations at finite temperature. *Physical Review Research*, **2020**, 2, | 3.9 | 23 |
| 78 | Van der Waals Interactions and Anharmonicity in the Lattice Vibrations, Dielectric Constants, Effective Charges, and Infrared Spectra of the Organic–Inorganic Halide Perovskite CH3NH3PbI3. *Journal of Physical Chemistry C*, **2017**, 121, 18459-18471 | 3.8 | 22 |
| 77 | O 1s core-level shifts at the anatase TiO2(101)/N3 photovoltaic interface: Signature of H-bonded supramolecular assembly. *Physical Review B*, **2011**, 84, | 3.3 | 22 |
| 76 | Single-Molecule Vibrational Spectroscopy of H2O on Anatase TiO2(101). *Journal of Physical Chemistry C*, **2017**, 121, 1182-1187 | 3.8 | 21 |

| | | | |
|---|---|---|---|
| 75 | Excitons in one-dimensional van der Waals materials: Sb2S3 nanoribbons. *Physical Review B*, **2015**, 92, | 3.3 | 21 |
| 74 | Equivalent oxide thickness of a thin oxide interlayer in gate insulator stacks on silicon. *Applied Physics Letters*, **2005**, 86, 192901 | 3.4 | 21 |
| 73 | Coexistence of Superconductivity with Enhanced Charge Density Wave Order in the Two-Dimensional Limit of TaSe. *Journal of Physical Chemistry Letters*, **2019**, 10, 4076-4081 | 6.4 | 20 |
| 72 | Proton-induced fixed positive charge at the Si(100)-SiO2 interface. *Physical Review Letters*, **2007**, 99, 126102 | 7.4 | 20 |
| 71 | Abrupt model interface for the 4H(1000)SiC-SiO2 interface. *Microelectronic Engineering*, **2005**, 80, 38-41 | 2.5 | 20 |
| 70 | Structural, electronic, elastic, power, and transport properties of □a2O3 from first principles. *Physical Review Research*, **2020**, 2, | 3.9 | 20 |
| 69 | Crossover from lattice to plasmonic polarons of a spin-polarised electron gas in ferromagnetic EuO. *Nature Communications*, **2018**, 9, 2305 | 17.4 | 19 |
| 68 | Spectral fingerprints of electron-plasmon coupling. *Physical Review B*, **2015**, 92, | 3.3 | 19 |
| 67 | Oxide Analogs of Halide Perovskites and the New Semiconductor BaAgIO. *Journal of Physical Chemistry Letters*, **2019**, 10, 1722-1728 | 6.4 | 18 |
| 66 | Universal Scaling of Intrinsic Resistivity in Two-Dimensional Metallic Borophene. *Angewandte Chemie - International Edition*, **2018**, 57, 4585-4589 | 16.4 | 18 |
| 65 | Mixed Wannier-Bloch functions for electrons and phonons in periodic systems. *Physical Review Letters*, **2006**, 96, 216403 | 7.4 | 17 |
| 64 | Modeling of Si 2p core-level shifts at Si□ZrO2)x(SiO2)1□ interfaces. *Applied Physics Letters*, **2002**, 81, 4233-4235 | 3.4 | 17 |
| 63 | Ruddlesden-Popper-Phase Hybrid Halide Perovskite/Small-Molecule Organic Blend Memory Transistors. *Advanced Materials*, **2021**, 33, e2003137 | 24 | 17 |
| 62 | Graphene Oxide/Perovskite Interfaces For Photovoltaics. *Journal of Physical Chemistry C*, **2018**, 122, 16715-16726 | 3.6 | 16 |
| 61 | High-Efficiency Fullerene Solar Cells Enabled by a Spontaneously Formed Mesostructured CuSCN-Nanowire Heterointerface. *Advanced Science*, **2018**, 5, 1700980 | 13.6 | 15 |
| 60 | Entangling remote nuclear spins linked by a chromophore. *Physical Review Letters*, **2010**, 104, 200501 | 7.4 | 15 |
| 59 | Role of fluorine in the iron pnictides: phonon softening and effective hole doping. *Physical Review Letters*, **2009**, 102, 147003 | 7.4 | 15 |
| 58 | Electron-plasmon and electron-phonon satellites in the angle-resolved photoelectron spectra of n-doped anatase TiO2. *Physical Review B*, **2018**, 97, | 3.3 | 14 |

| | | | |
|---|---|---|---|
| 57 | Time-dependent density functional theory using atomic orbitals and the self-consistent Sternheimer equation. *Physical Review B*, **2014**, 89, | 3.3 | 14 |
| 56 | Limits to Electrical Mobility in Lead-Halide Perovskite Semiconductors. *Journal of Physical Chemistry Letters*, **2021**, 12, 3607-3617 | 6.4 | 14 |
| 55 | The GW plus cumulant method and plasmonic polarons: application to the homogeneous electron gas*. *European Physical Journal B*, **2016**, 89, 1 | 1.2 | 14 |
| 54 | Ab initio calculation of spin fluctuation spectra using time-dependent density functional perturbation theory, plane waves, and pseudopotentials. *Physical Review B*, **2018**, 97, | 3.3 | 13 |
| 53 | Theory of Electromagnons in CuO. *Physical Review Letters*, **2015**, 114, 197201 | 7.4 | 13 |
| 52 | Linear optical response of finite systems using multishift linear system solvers. *Journal of Chemical Physics*, **2014**, 141, 044117 | 3.9 | 13 |
| 51 | First-principles study of structurally modulated multiferroic CaMn7O12. *Physical Review B*, **2015**, 91, | 3.3 | 12 |
| 50 | Dielectric screening in extended systems using the self-consistent Sternheimer equation and localized basis sets. *Physical Review B*, **2012**, 85, | 3.3 | 12 |
| 49 | Phonon-Limited Mobility and Electron-Phonon Coupling in Lead-Free Halide Double Perovskites. *Journal of Physical Chemistry Letters*, **2021**, 12, 4474-4482 | 6.4 | 12 |
| 48 | Atomic Structure of Water Monolayer on Anatase TiO2(101) Surface. *Journal of Physical Chemistry C* , **2018**, 122, 11954-11960 | 3.8 | 12 |
| 47 | Quasiparticle GW band structures and Fermi surfaces of bulk and monolayer NbS2. *Physical Review B*, **2018**, 98, | 3.3 | 10 |
| 46 | Intrinsic quantum confinement in formamidinium lead triiodide perovskite. *Nature Materials*, **2020**, 19, 1201-1206 | 27 | 10 |
| 45 | Slot-Die-Printed Two-Dimensional ZrS Charge Transport Layer for Perovskite Light-Emitting Diodes. *ACS Applied Materials & Interfaces*, **2019**, 11, 48021-48028 | 9.5 | 10 |
| 44 | Crystallographic, Optical, and Electronic Properties of the Cs2AgBi1−xInxBr6 Double Perovskite: Understanding the Fundamental Photovoltaic Efficiency Challenges. *ACS Energy Letters*, **2021**, 6, 1073-1081 | 20.1 | 10 |
| 43 | Manipulating surface magnetic order in iron telluride. *Science Advances*, **2019**, 5, eaav3478 | 14.3 | 9 |
| 42 | First-principles investigation of hyperfine interactions for nuclear spin entanglement in photoexcited fullerenes. *Physical Review B*, **2012**, 85, | 3.3 | 9 |
| 41 | Dose and dose-rate effects on NPN bipolar junction transistors irradiated at high temperature. *IEEE Transactions on Nuclear Science*, **2002**, 49, 1474-1479 | 1.7 | 8 |
| 40 | Electron-polaron dichotomy of charge carriers in perovskite oxides. *Communications Physics*, **2020**, 3, | 5.4 | 7 |

| | | | |
|---|---|---|---|
| 39 | Energy-level alignment and open-circuit voltage at graphene/polymer interfaces: theory and experiment. *2D Materials*, **2016**, 3, 015003 | 5.9 | 7 |
| 38 | Infrared properties of ultrathin oxides on Si(100). *Microelectronic Engineering*, **2005**, 80, 420-423 | 2.5 | 7 |
| 37 | SternheimerGW: A program for calculating GW quasiparticle band structures and spectral functions without unoccupied states. *Computer Physics Communications*, **2020**, 247, 106856 | 4.2 | 7 |
| 36 | Performance of local orbital basis sets in the self-consistent Sternheimer method for dielectric matrices of extended systems. *European Physical Journal B*, **2012**, 85, 1 | 1.2 | 6 |
| 35 | First-principles theory of infrared absorption spectra at surfaces and interfaces: Application to the Si(100):H2O surface. *Physical Review B*, **2008**, 78, | 3.3 | 6 |
| 34 | Electronic Structure at Realistic Si(100)-SiO2Interfaces. *Japanese Journal of Applied Physics*, **2004**, 43, 7895-7898 | 1.4 | 6 |
| 33 | Monolayer 1T-NbSe as a 2D-correlated magnetic insulator. *Science Advances*, **2021**, 7, eabi6339 | 14.3 | 6 |
| 32 | First-principles study of multiferroic RbFe(MoO4)2. *Physical Review B*, **2014**, 90, | 3.3 | 5 |
| 31 | Publisher Note: First-Principles Prediction of Doped Graphane as a High-Temperature Electron-Phonon Superconductor [Phys. Rev. Lett. 105, 037002 (2010)]. *Physical Review Letters*, **2010**, 105, | 7.4 | 5 |
| 30 | Multiphonon diffuse scattering in solids from first principles: Application to layered crystals and two-dimensional materials. *Physical Review B*, **2021**, 104, | 3.3 | 5 |
| 29 | Efficient First-Principles Methodology for the Calculation of the All-Phonon Inelastic Scattering in Solids. *Physical Review Letters*, **2021**, 127, 207401 | 7.4 | 5 |
| 28 | First-principles predictions of Hall and drift mobilities in semiconductors. *Physical Review Research*, **2021**, 3, | 3.9 | 5 |
| 27 | Quasiparticle Band Structure and Phonon-Induced Band Gap Renormalization of the Lead-Free Halide Double Perovskite Cs2InAgCl6. *Journal of Physical Chemistry C*, | 3.8 | 5 |
| 26 | Universal Scaling of Intrinsic Resistivity in Two-Dimensional Metallic Borophene. *Angewandte Chemie*, **2018**, 130, 4675-4679 | 3.6 | 4 |
| 25 | Hybrid Halide Perovskites: Fundamental Theory and Materials Design **2018**, 1-30 | | 4 |
| 24 | Inelastic carrier lifetime in bilayer graphene. *Applied Physics Letters*, **2012**, 100, 032106 | 3.4 | 4 |
| 23 | Exciton-Phonon Interactions in Monolayer Germanium Selenide from First Principles. *Journal of Physical Chemistry Letters*, **2021**, 12, 3802-3808 | 6.4 | 4 |
| 22 | Spin waves in metallic iron and nickel measured by soft x-ray resonant inelastic scattering. *Physical Review B*, **2020**, 102, | 3.3 | 3 |

| | | | |
|---|---|---|---|
| 21 | Superconducting properties of MoTe2 from ab initio anisotropic Migdal-Eliashberg theory. *Physical Review B*, **2020**, 101, | 3.3 | 3 |
| 20 | Many-body renormalization of the electron effective mass of InSe. *Physical Review B*, **2020**, 101, | 3.3 | 3 |
| 19 | Model for high-temperature radiation effects in n-p-n bipolar-junction transistors. *IEEE Transactions on Nuclear Science*, **2002**, 49, 2990-2997 | 1.7 | 3 |
| 18 | Electronic Structure and Electron-Transport Properties of Three Metal Hexacyanoferrates. *Chemistry of Materials*, **2021**, 33, 7067-7074 | 9.6 | 3 |
| 17 | Hybrid Halide Perovskites: Fundamental Theory and Materials Design **2020**, 295-324 | | 2 |
| 16 | Theory and Computation of Hall Scattering Factor in Graphene. *Nano Letters*, **2020**, 20, 8861-8865 | 11.5 | 2 |
| 15 | CeTaN3 and CeNbN3: Prospective Nitride Perovskites with Optimal Photovoltaic Band Gaps. *Chemistry of Materials*, **2022**, 34, 2107-2122 | 9.6 | 2 |
| 14 | Trellises of Molecular Oxygen on Anatase TiO2(101). *Journal of Physical Chemistry C*, **2019**, 123, 26170-26177 | 3.7 | 1 |
| 13 | Solar Cells: Structural and Electronic Properties of Semiconductor-Sensitized Solar-Cell Interfaces (Adv. Funct. Mater. 24/2011). *Advanced Functional Materials*, **2011**, 21, 4798-4798 | 15.6 | 1 |
| 12 | Modeling the role of the fluorine dopant in the magnetic phase diagram of LaFeAsO1−xFx superconductors. *Physical Review B*, **2012**, 85, | 3.3 | 1 |
| 11 | Dose and dose rate effects on NPN bipolar junction transistors irradiated at high temperature | | 1 |
| 10 | Dynamic Rashba-Dresselhaus Effect.. *Physical Review Letters*, **2021**, 127, 237601 | 7.4 | 1 |
| 9 | GW band structure of monolayer MoS2 using the SternheimerGW method and effect of dielectric environment. *Physical Review B*, **2021**, 103, | 3.3 | 1 |
| 8 | Modelling graphene quantum dot functionalization via ethylene-dinitrobenzoyl. *Applied Physics Letters*, **2016**, 108, 123902 | 3.4 | 1 |
| 7 | Halide Perovskites: Interfaces Between Graphene-Related Materials and MAPbI3: Insights from First-Principles (Adv. Mater. Interfaces 22/2018). *Advanced Materials Interfaces*, **2018**, 5, 1870110 | 4.6 | 1 |
| 6 | First-principles study of electron transport in ScN. *Physical Review B*, **2021**, 104, | 3.3 | 1 |
| 5 | DIELECTRIC AND INFRARED PROPERTIES OF ULTRATHIN SiO2 LAYERS ON Si(100). *NATO Science Series Series II, Mathematics, Physics and Chemistry*, **2006**, 385-396 | | 1 |
| 4 | Ultrafast photo-induced phonon hardening due to Pauli blocking in MAPbI3 single-crystal and polycrystalline perovskites. *JPhys Materials*, **2021**, 4, 044017 | 4.2 | 0 |

# List of Publications

3 Atomic-scale investigation of the dielectric screening at the interface between silicon and its oxide. *Materials Research Society Symposia Proceedings*, **2003**, 786, 511

2 Many-Body Calculations of Plasmon and Phonon Satellites in Angle-Resolved Photoelectron Spectra Using the Cumulant Expansion Approach **2020**, 341-365

1 Many-Body Calculations of Plasmon and Phonon Satellites in Angle-Resolved Photoelectron Spectra Using the Cumulant Expansion Approach **2018**, 1-25