# Emilio Artacho

List of Publications by Year
in descending order

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|---|---|---|---|
| 192 papers | 25,708 citations | 25034 57 h-index | 6131 159 g-index |
| 197 all docs | 197 docs citations | 197 times ranked | 17425 citing authors |

| # | Article | IF | Citations |
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| 1 | Manifold curvature and Ehrenfest forces with a moving basis. SciPost Physics, 2022, 12, . | 4.9 | 0 |
| 2 | Bragg's additivity rule and core and bond model studied by real-time TDDFT electronic stopping simulations: The case of water vapor. Radiation Physics and Chemistry, 2022, 193, 109961. | 2.8 | 2 |
| 3 | Semi-empirical and linear-scaling DFT methods to characterize duplex DNA and G-quadruplexes in the presence of interacting small molecules. Physical Chemistry Chemical Physics, 2022, 24, 11510-11519. | 2.8 | 5 |
| 4 | Inelastic scattering of electrons in water from first principles: cross sections and inelastic mean free path for use in Monte Carlo track-structure simulations of biological damage. Royal Society Open Science, 2022, 9, . | 2.4 | 4 |
| 5 | Local orbital formulation of the Floquet theory of projectile electronic stopping. Physical Review B, 2022, 105, . | 3.2 | 1 |
| 6 | Numerical integration of quantum time evolution in a curved manifold. Physical Review Research, 2021, 3, . | 3.6 | 2 |
| 7 | The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117. | 3.0 | 19 |
| 8 | Efficient ab initio calculation of electronic stopping in disordered systems via geometry pre-sampling: Application to liquid water. Journal of Chemical Physics, 2020, 153, 034113. | 3.0 | 7 |
| 9 | Changing the paradigm for research publishing. Physics Today, 2020, 73, 10-10. | 0.3 | 0 |
| 10 | S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108. | 3.0 | 229 |
| 11 | Gap variability upon packing in organic photovoltaics. PLoS ONE, 2020, 15, e0234115. | 2.5 | 0 |
| 12 | Entropic bonding of the type 1 pilus from experiment and simulation. Royal Society Open Science, 2020, 7, 200183. | 2.4 | 0 |
| 13 | Ab initio electronic stopping power for protons in Ga <sub>0.5</sub> In <sub>0.5</sub> P/GaAs/Ge triple-junction solar cells for space applications. Royal Society Open Science, 2020, 7, 200925. | 2.4 | 9 |
| 14 | First-principles characterization of single-electron polaron in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml | 3.6 | 15 |
| | Physical Review Research, 2020, 2, . | | |
| 15 | Floquet theory for the electronic stopping of projectiles in solids. Physical Review Research, 2020, 2, . | 3.6 | 4 |
| 16 | Electrostatics and domains in ferroelectric superlattices. Royal Society Open Science, 2020, 7, 201270. | 2.4 | 12 |
| 17 | Electronic heat transport versus atomic heating in irradiated short metallic nanowires. Physical Review B, 2019, 100, . | 3.2 | 6 |
| 18 | Anisotropy of electronic stopping power in graphite. Physical Review B, 2019, 100, . | 3.2 | 19 |

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| 19 | Prediction of the near-IR spectra of ices by ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2019, 21, 9433-9440. | 2.8 | 2 |
| 20 | Comparison of dispersion-corrected exchange-correlation functionals using atomic orbitals. Physical Review B, 2019, 100, . | 3.2 | 5 |
| 21 | Prediction of equilibrium isotopic fractionation of the gypsum/bassanite/water system using first-principles calculations. Geochimica Et Cosmochimica Acta, 2019, 244, 1-11. | 3.9 | 9 |
| 22 | Dynamical continuum simulation of condensed matter from first principles. Physical Review Research, 2019, 1, . | 3.6 | 0 |
| 23 | Bulk properties and near-critical behaviour of SiO2 fluid. Earth and Planetary Science Letters, 2018, 491, 11-20. | 4.4 | 10 |
| 24 | Core Electrons in the Electronic Stopping of Heavy Ions. Physical Review Letters, 2018, 121, 116401. | 7.8 | 72 |
| 25 | Mechanical architecture and folding of E. coli type 1 pilus domains. Nature Communications, 2018, 9, 2758. | 12.8 | 55 |
| 26 | Effect of magnetism and temperature on the stability of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:msub><mm phases. Physical Review Materials, 2018, 2, . | 2.4 | 1 |
| 27 | Simulations and spectra of water in CO matrices. Physical Chemistry Chemical Physics, 2017, 19, 7280-7287. | 2.8 | 1 |
| 28 | Quantum mechanics in an evolving Hilbert space. Physical Review B, 2017, 95, . | 3.2 | 16 |
| 29 | Stopping power beyond the adiabatic approximation. Scientific Reports, 2017, 7, 2618. | 3.3 | 77 |
| 30 | Simulations of water nano-confined between corrugated planes. Journal of Chemical Physics, 2017, 147, 194509. | 3.0 | 7 |
| 31 | Water radiolysis by low-energy carbon projectiles from first-principles molecular dynamics. PLoS ONE, 2017, 12, e0171820. | 2.5 | 10 |
| 32 | Structural and configurational properties of nanoconfined monolayer ice from first principles. Scientific Reports, 2016, 6, 18651. | 3.3 | 61 |
| 33 | <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="italic">Ab</mml:mi></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="italic">initio</mml:mi></mml:math>calculation of the shock Hugoniot of bulk silicon. Physical Review B, 2016, 93, . | 3.2 | 14 |
| 34 | Electronic and magnetic properties of superconductingLnO<sub>1â”’x</sub>F<sub>x</sub>BiS<sub>2</sub>(Lnâ€‰â€‰â€‰â€‰a,) Tj ETQ | | |
| 35 | Continuous melting through a hexatic phase in confined bilayer water. Physical Review E, 2016, 93, 062137. | 2.1 | 15 |
| 36 | Enhanced Configurational Entropy in High-Density Nanoconfined Bilayer Ice. Physical Review Letters, 2016, 116, 085901. | 7.8 | 42 |

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| 37 | Electronic stopping power in a narrow band gap semiconductor from first principles. Physical Review B, 2015, 91, . | 3.2 | 57 |
| 38 | Fermi surfaces and orbital polarization in superconducting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CeO</mml:mi><mml:mrow><mml:mn>0.5</ mathvariant="normal">F</mml:mi><mml:mrow><mml:mn>0.5</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi>BiS</mml:m by angle-resolved photoemission spectroscopy. Physical Review B, 2015, 92, . | 3.2 | 36 |
| 39 | Two-dimensional electron gas at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>PbTi</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>/</mml:mo><mml:mi>SrTi</mml:mi><mml:msub><mml: mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>interface: An ab initio study. Physical Review B, 2015, 92, . | 3.2 | 34 |
| 40 | Electronic structure predictions in Bi-O-S systems. Novel Superconducting Materials, 2015, 1, . | 0.8 | 0 |
| 41 | Model of two-dimensional electron gas formation at ferroelectric interfaces. Physical Review B, 2015, 92, . | 3.2 | 30 |
| 42 | Effects of stoichiometric doping in superconducting Bi-O-S compounds. Journal of Physics Condensed Matter, 2015, 27, 135501. | 1.8 | 13 |
| 43 | Species fractionation in atomic chains from mechanically stretched alloys. Journal of Physics Condensed Matter, 2014, 26, 435304. | 1.8 | 0 |
| 44 | The origin of two-dimensional electron gases at oxide interfaces: insights from theory. Journal of Physics Condensed Matter, 2014, 26, 143201. | 1.8 | 140 |
| 45 | Room temperature compressibility and diffusivity of liquid water from first principles. Journal of Chemical Physics, 2013, 139, 194502. | 3.0 | 54 |
| 46 | Knock-on damage in bilayer graphene: Indications for a catalytic pathway. Physical Review B, 2013, 88, . | 3.2 | 19 |
| 47 | Electronic stopping power of H and He in Al and LiF from first principles. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 59-61. | 1.4 | 32 |
| 48 | One-dimensional half-metallic interfaces of two-dimensional honeycomb insulators. Physical Review B, 2013, 88, . | 3.2 | 28 |
| 49 | Optimal finite-range atomic basis sets for liquid water and ice. Journal of Physics Condensed Matter, 2013, 25, 435504. | 1.8 | 25 |
| 50 | Proposal of a One-Dimensional Electron Gas in the Steps at the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LaAlO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Interf Physical Review Letters, 2012, 108, 166802. | 7.8 | 21 |
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| 52 | Molecular and Electronic Structure of the Peptide Subunit of Geobacter sulfurreducens Conductive Pili from First Principles. Journal of Physical Chemistry A, 2012, 116, 8023-8030. | 2.5 | 58 |
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| 57 | van der Waals interaction in magnetic bilayer graphene nanoribbons. Physical Review B, 2012, 85, . | 3.2 | 41 |
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| 59 | Density, structure, and dynamics of water: The effect of van der Waals interactions. Journal of Chemical Physics, 2011, 134, 024516. | 3.0 | 242 |
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| 61 | The net charge at interfaces between insulators. Journal of Physics Condensed Matter, 2011, 23, 081001. | 1.8 | 18 |
| 62 | Surface defects and conduction in polar oxide heterostructures. Physical Review B, 2011, 83, . | 3.2 | 145 |
| 63 | Comment on â€œQuantum Mechanics in Metric Space: Wave Functions and their Densitiesâ€• Physical Review Letters, 2011, 107, 188901; discussion 188902. | 7.8 | 4 |
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| 78 | First-principles molecular dynamics simulations of the interaction of ionic projectiles with liquid water and ice. , 2008, , . | | 8 |
| 79 | Electrostatic versus polarization effects in the adsorption of aromatic molecules of varied polarity on an insulating hydrophobic surface. Journal of Physics Condensed Matter, 2008, 20, 035215. | 1.8 | 16 |
| 80 | First-principles calculations of structural changes in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>B</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mtext> under pressure. Physical Review B, 2008, 78, . | 3.2 | 22 |
| 81 | Ferrielectric Twin Walls in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 097602. | 7.8 | 148 |
| 82 | Nature of the Structural Transformations in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Glass under High Pressure. Physical Review Letters, 2008, 101, 035702. | 7.8 | 76 |
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| 92 | Electrons and Hydrogen-Bond Connectivity in Liquid Water. Physical Review Letters, 2006, 96, 016404. | 7.8 | 88 |
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| 110 | Intrinsic point defects and volume swelling inZrSiO4under irradiation. Physical Review B, 2004, 70, . | 3.2 | 24 |
| 111 | Density-functional study of charge doping inWO3. Physical Review B, 2004, 70, . | 3.2 | 84 |
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