# Gustavo M Dalpian

List of Publications by Year
in descending order

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Version: 2024-02-01

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|---|---|---|---|
| 96 papers | 2,962 citations | 186265 28 h-index | 175258 52 g-index |
| 96 all docs | 96 docs citations | 96 times ranked | 4134 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Intrinsic doping limitations in inorganic lead halide perovskites. Materials Horizons, 2022, 9, 791-803. | 12.2 | 10 |
| 2 | Machine Learning Study of the Magnetic Ordering in 2D Materials. ACS Applied Materials & Interfaces, 2022, 14, 9418-9432. | 8.0 | 35 |
| 3 | Pressure-Induced Stabilization of Sodium Halide Perovskites. Journal of Physical Chemistry C, 2022, 126, 4248-4254. | 3.1 | 0 |
| 4 | High-throughput inverse design and Bayesian optimization of functionalities: spin splitting in two-dimensional compounds. Scientific Data, 2022, 9, 195. | 5.3 | 2 |
| 5 | Hole conductivity through a defect band in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>ZnGa</mml:mi></mml:mrow><mml:mn>2</ mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review Materials, 2022, 6, . | 2.4 | 4 |
| 6 | Entropy-driven stabilization of the cubic phase of MaPbI<sub>3</sub> at room temperature. Journal of Materials Chemistry A, 2021, 9, 1089-1099. | 10.3 | 35 |
| 7 | Ab initio atomistic description of temperature-induced phase changes: The cases of zirconia and Ti-Y-co-doped zirconia. Physical Review Materials, 2021, 5, . | 2.4 | 2 |
| 8 | MXene Phase with C<sub>3</sub> Structure Unit: A Family of 2D Electrides. Advanced Functional Materials, 2021, 31, 2100009. | 14.9 | 13 |
| 9 | Tailoring the Optical, Electronic, and Magnetic Properties of MAPbI<sub>3</sub> through Self-Assembled Fe Incorporation. Journal of Physical Chemistry C, 2021, 125, 15636-15646. | 3.1 | 9 |
| 10 | Different shapes of spin textures as a journey through the Brillouin zone. Physical Review B, 2021, 104, . | 3.2 | 23 |
| 11 | Influence of defects on antidoping behavior in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Sm</mml:mi><mml:mi>Ni</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2021, 104, . | 3.2 | 6 |
| 12 | Realization of predicted exotic materials: The burden of proof. Materials Today, 2020, 32, 35-45. | 14.2 | 29 |
| 13 | Ab Initio Simulations and Materials Chemistry in the Age of Big Data. Journal of Chemical Information and Modeling, 2020, 60, 452-459. | 5.4 | 28 |
| 14 | The Rashba Scale: Emergence of Band Anti-crossing as a Design Principle for Materials with Large Rashba Coefficient. Matter, 2020, 3, 145-165. | 10.0 | 21 |
| 15 | Doping quantum materials: Defects and impurities in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Fe</mml:mi><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi><mml:m Physical Review B, 2020, 102, . | 3.2 | 5 |
| 16 | Inverse design of compounds that have simultaneously ferroelectric and Rashba cofunctionality. Physical Review B, 2020, 102, . | 3.2 | 20 |
| 17 | Iron and oxygen vacancies at the hematite surface: pristine case and with a chlorine adatom. Physical Chemistry Chemical Physics, 2020, 22, 25380-25389. | 2.8 | 7 |
| 18 | Insulatorâ€“Metal Transition in the Nd<sub>2</sub>CoFeO<sub>6</sub> Disordered Double Perovskite. Journal of Physical Chemistry C, 2020, 124, 22733-22742. | 3.1 | 5 |

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|---|---|---|---|
| 19 | Electronic mechanism for resistive switching in metal/insulator/metal nanodevices. Journal Physics D: Applied Physics, 2020, 53, 295302. | 2.8 | 1 |
| 20 | Polymorphous nature of cubic halide perovskites. Physical Review B, 2020, 101, . | 3.2 | 104 |
| 21 | Possible Charge-Transfer-Induced Conductivity Enhancement in TiO<sub>2</sub> Microtubes Decorated with Perovskite CsPbBr<sub>3</sub> Nanocrystals. Langmuir, 2020, 36, 5408-5416. | 3.5 | 5 |
| 22 | Tuning hydrogen adsorption and electronic properties from graphene to fluorographone. Physical Review Materials, 2020, 4, . | 2.4 | 5 |
| 23 | Spins in Semiconductor Nanocrystals. , 2020, , 605-616. | | 0 |
| 24 | Preface to the Forum on Materials Discovery and Design. ACS Applied Materials & Interfaces, 2019, 11, 24823-24824. | 8.0 | 3 |
| 25 | Zeeman-type spin splitting in nonmagnetic three-dimensional compounds. Npj Quantum Materials, 2019, 4, . | 5.2 | 23 |
| 26 | Antidoping in Insulators and Semiconductors Having Intermediate Bands with Trapped Carriers. Physical Review Letters, 2019, 122, 106403. | 7.8 | 28 |
| 27 | Formation and Composition-Dependent Properties of Alloys of Cubic Halide Perovskites. Chemistry of Materials, 2019, 31, 2497-2506. | 6.7 | 48 |
| 28 | Controlling the Activation Energy for Single-Ion Diffusion through a Hybrid Polyelectrolyte Matrix by Manipulating the Central Coordinate Semimetal Atom. Journal of Physical Chemistry Letters, 2019, 10, 7684-7689. | 4.6 | 0 |
| 29 | Computational screening of bulk materials with intrinsic intermediate band. Computational Materials Science, 2019, 158, 382-388. | 3.0 | 10 |
| 30 | Semiclassical transport properties of IrGa<sub>3</sub>: a promising thermoelectric material. Journal of Physics Condensed Matter, 2018, 30, 085701. | 1.8 | 7 |
| 31 | Interaction of Water with the Gypsum (010) Surface: Structure and Dynamics from Nonlinear Vibrational Spectroscopy and Ab Initio Molecular Dynamics. Journal of the American Chemical Society, 2018, 140, 17141-17152. | 13.7 | 19 |
| 32 | Spins in Semiconductor Nanocrystals. , 2018, , 1-12. | | 0 |
| 33 | Bond disproportionation, charge self-regulation, and ligand holes in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>s</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>p</mml:mi></mml:mrow></mml:math> and in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math> -electron <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>A</mml:mi><mml:mi>B</mml:mi><mml:mi> | 3.2 | 45 |
| 34 | Oxidation of free-standing and supported borophene. 2D Materials, 2017, 4, 025025. | 4.4 | 31 |
| 35 | High temperature activation of hematite nanorods for sunlight driven water oxidation reaction. Physical Chemistry Chemical Physics, 2017, 19, 25025-25032. | 2.8 | 23 |
| 36 | Surface Fe vacancy defects on haematite and their role in light-induced water splitting in artificial photosynthesis. Physical Chemistry Chemical Physics, 2017, 19, 31410-31417. | 2.8 | 12 |

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| 37 | Changes in charge density vs changes in formal oxidation states: The case of Sn halide perovskites and their ordered vacancy analogues. Physical Review Materials, 2017, 1, . | 2.4 | 43 |
| 38 | Vacancies at LaAlO3 thin films: A 2D electron gas at the surface. Journal of Alloys and Compounds, 2016, 684, 544-548. | 5.5 | 8 |
| 39 | Emergence of competing magnetic interactions induced by Ge doping in the semiconductorFeGa3. Physical Review B, 2016, 94, . | 3.2 | 9 |
| 40 | Charge storage in oxygen deficient phases of TiO2: defect Physics without defects. Scientific Reports, 2016, 6, 28871. | 3.3 | 48 |
| 41 | Effect of Charges on the Interaction of a Water Molecule with the Fe<sub>2</sub>O<sub>3</sub>(0001) Surface. Journal of Physical Chemistry C, 2016, 120, 11918-11925. | 3.1 | 22 |
| 42 | A search for the ground state structure and the phase stability of tantalum pentoxide. Journal of Physics Condensed Matter, 2016, 28, 035801. | 1.8 | 27 |
| 43 | <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>Simu of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ti</mml:mi></mml:mrow><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>7</mml:mn></mml:mrow></mml:msub><mml:mtext>â^’</mml:mtext></mml:mrow></mml:math>Physical Review Applied, 2015, 3, . | 3.8 | 15 |
| 44 | A systematic first-principles study of the tungsten trioxide polymorphs. Physica Status Solidi (B): Basic Research, 2015, 252, 2290-2295. | 1.5 | 2 |
| 45 | <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Ti</mml:mi><mml:mi>n</mml:mi></mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn><mml:mi>n</mml:mi><mml:mo>â^’</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:math> phases studied using density functional theory. Physical Review B, 2014, 90, . | 3.2 | 33 |
| 46 | Oxygen vacancies at the surface of SrTiO<sub>3</sub> thin films. Journal of Applied Physics, 2014, 115, 033710. | 2.5 | 14 |
| 47 | First principles investigations on the electronic structure of anchor groups on ZnO nanowires and surfaces. Journal of Applied Physics, 2014, 115, . | 2.5 | 16 |
| 48 | First-principles equation of state and phase stability of niobium pentoxide. Computational Materials Science, 2014, 81, 133-140. | 3.0 | 59 |
| 49 | Cobalt-doped ZnO nanocrystals: quantum confinement and surface effects from ab initio methods. Physical Chemistry Chemical Physics, 2013, 15, 15863. | 2.8 | 12 |
| 50 | Electronic, dielectric, and optical properties of the B phase of niobium pentoxide and tantalum pentoxide by firstâ€principles calculations. Physica Status Solidi (B): Basic Research, 2013, 250, 1644-1650. | 1.5 | 24 |
| 51 | Conduction electron spin resonance in AlB<sub>2</sub>. Journal of Physics Condensed Matter, 2013, 25, 216001. | 1.8 | 5 |
| 52 | Pressure-induced metal-insulator transition and absence of magnetic order in FeGa<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>from a first-principles study. Physical Review B, 2012, 86, . | 3.2 | 19 |
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| 54 | Computational studies of doped nanostructures. Reports on Progress in Physics, 2011, 74, 046501. | 20.1 | 52 |

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| 55 | First-principles calculations of lattice-strained core-shell nanocrystals. Physical Review B, 2011, 84, . | 3.2 | 21 |
| 56 | Liquid separation by a graphene membrane. Journal of Applied Physics, 2010, 108, 113527. | 2.5 | 14 |
| 57 | Origin of FM Ordering in Pristine Micro- and Nanostructured ZnO. Nano Letters, 2010, 10, 1383-1386. | 9.1 | 98 |
| 58 | Surface and Quantum Confinement Effects in ZnO Nanocrystals. Journal of Physical Chemistry C, 2010, 114, 18293-18297. | 3.1 | 53 |
| 59 | Role of Confinement on Diffusion Barriers in Semiconductor Nanocrystals. Physical Review Letters, 2009, 102, 025901. | 7.8 | 27 |
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| 61 | Evidence for a subtle structural symmetry breaking in EuB<sub>6</sub>. Journal of Physics Condensed Matter, 2009, 21, 456007. | 1.8 | 9 |
| 62 | Surface magnetization in non-doped ZnO nanostructures. Applied Physics Letters, 2009, 94, . | 3.3 | 74 |
| 63 | Effects of Side-Chain and Electron Exchange Correlation on the Band Structure of Perylene Diimide Liquid Crystals: A Density Functional Study. Journal of Physical Chemistry B, 2009, 113, 5376-5380. | 2.6 | 12 |
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| 65 | Quantum confinement effects on Mn-doped InAs nanocrystals: A first-principles study. Physical Review B, 2008, 78, . | 3.2 | 18 |
| 66 | Carrier-induced enhancement and suppression of ferromagnetism in Zn<sub>1-x</sub>Cr<sub>x</sub>Te and Ga<sub>1-x</sub>Cr<sub>x</sub>As: origin of the spinodal decomposition. New Journal of Physics, 2008, 10, 113007. | 2.9 | 8 |
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| 69 | Symmetry Considerations in CdSe Nanocrystals. Nano Letters, 2006, 6, 501-504. | 9.1 | 31 |
| 70 | Self-Purification in Semiconductor Nanocrystals. Physical Review Letters, 2006, 96, 226802. | 7.8 | 613 |
| 71 | Energetic Pinning of Magnetic Impurity Levels in Quantum-Confined Semiconductors. Nano Letters, 2006, 6, 2887-2892. | 9.1 | 45 |
| 72 | Study of Phase Selectivity of Organicâ"Inorganic Hybrid Semiconductors. Chemistry of Materials, 2006, 18, 2805-2809. | 6.7 | 35 |

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| 73 | Carrier-mediated stabilization of ferromagnetism in semiconductors: holes and electrons. Physica Status Solidi (B): Basic Research, 2006, 243, 2170-2187. | 1.5 | 46 |
| 74 | Phenomenological band structure model of magnetic coupling in semiconductors. Solid State Communications, 2006, 138, 353-358. | 1.9 | 134 |
| 75 | Novel Approach to Tuning the Physical Properties of Organic-Inorganic Hybrid Semiconductors. Physical Review Letters, 2006, 96, 026405. | 7.8 | 52 |
| 76 | Impurity-induced phase stabilization of semiconductors. Applied Physics Letters, 2006, 89, 011907. | 3.3 | 20 |
| 77 | Electron-mediated ferromagnetism and negativesâˆ’dexchange splitting in semiconductors. Physical Review B, 2006, 73, . | 3.2 | 23 |
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| 81 | First-principles study of Mn-induced local magnetic moments in host semiconductors. Physical Review B, 2005, 71, . | 3.2 | 23 |
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| 85 | Hole-Mediated Stabilization of Cubic GaN. Physical Review Letters, 2004, 93, 216401. | 7.8 | 32 |
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| 87 | Energetics and electronic structure of stacking faults in ZnO. Physical Review B, 2004, 70, . | 3.2 | 85 |
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| 91 | Influence of surface degrees of freedom on the adsorption of Ge ad-atoms on Si(100). Computational Materials Science, 2001, 22, 19-23. | 3.0 | 0 |
| 92 | Theoretical STM images of Ge monomers and trimers on Si(100). Surface Science, 2001, 482-485, 507-511. | 1.9 | 0 |
| 93 | Adsorption of monomers on semiconductors and the importance of surface degrees of freedom. Physical Review B, 2001, 63, . | 3.2 | 8 |
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| 95 | Two-Atom Structures of Ge on Si(100): Dimers versus Adatom Pairs. Physical Review Letters, 2001, 87, 036104. | 7.8 | 5 |
| 96 | Initial stages of Ge growth on Si(100): ad-atoms, ad-dimers, and ad-trimers. Physica B: Condensed Matter, 1999, 273-274, 589-592. | 2.7 | 10 |