Gustavo M Dalpian

List of Publications by Year
in descending order

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	Self-Purification in Semiconductor Nanocrystals. Physical Review Letters, 2006, 96, 226802.	7.8	613
2	Phenomenological band structure model of magnetic coupling in semiconductors. Solid State Communications, 2006, 138, 353-358.	1.9	134
3	Electron-induced stabilization of ferromagnetism inGa1â^'xGdxN. Physical Review B, 2005, 72, .	3.2	120
4	Polymorphous nature of cubic halide perovskites. Physical Review B, 2020, 101, .	3.2	104
5	Origin of FM Ordering in Pristine Micro- and Nanostructured ZnO. Nano Letters, 2010, 10, 1383-1386.	9.1	98
6	Energetics and electronic structure of stacking faults in ZnO. Physical Review B, 2004, 70, .	3.2	85
7	Surface magnetization in non-doped ZnO nanostructures. Applied Physics Letters, 2009, 94, .	3.3	74
8	Barrier-free substitutional doping of graphene sheets with boron atoms:Ab initiocalculations. Physical Review B, 2009, 79, .	3.2	63
9	First-principles equation of state and phase stability of niobium pentoxide. Computational Materials Science, 2014, 81, 133-140.	3.0	59
10	Ab initiodetermination of the atomistic structure ofSixGe1â^'xalloy. Physical Review B, 2001, 64, .	3.2	57
11	Surface and Quantum Confinement Effects in ZnO Nanocrystals. Journal of Physical Chemistry C, 2010, 114, 18293-18297.	3.1	53
12	Novel Approach to Tuning the Physical Properties of Organic-Inorganic Hybrid Semiconductors. Physical Review Letters, 2006, 96, 026405.	7.8	52
13	Computational studies of doped nanostructures. Reports on Progress in Physics, 2011, 74, 046501.	20.1	52
14	Charge storage in oxygen deficient phases of TiO2: defect Physics without defects. Scientific Reports, 2016, 6, 28871.	3.3	48
15	Formation and Composition-Dependent Properties of Alloys of Cubic Halide Perovskites. Chemistry of Materials, 2019, 31, 2497-2506.	6.7	48
16	Carrier-mediated stabilization of ferromagnetism in semiconductors: holes and electrons. Physica Status Solidi (B): Basic Research, 2006, 243, 2170-2187.	1.5	46
17	Energetic Pinning of Magnetic Impurity Levels in Quantum-Confined Semiconductors. Nano Letters, 2006, 6, 2887-2892.	9.1	45
18	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

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19	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
20	Theoretical investigation of a possibleMnxSi1â^'xferromagnetic semiconductor. Physical Review B, 2003, 68, .	3.2	42
21	Study of Phase Selectivity of Organicâ^'Inorganic Hybrid Semiconductors. Chemistry of Materials, 2006, 18, 2805-2809.	6.7	35
22	Entropy-driven stabilization of the cubic phase of MaPbI₃ at room temperature. Journal of Materials Chemistry A, 2021, 9, 1089-1099.	10.3	35
23	Machine Learning Study of the Magnetic Ordering in 2D Materials. ACS Applied Materials & Interfaces, 2022, 14, 9418-9432.	8.0	35
24	<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:ms mathvariant="normal">O</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mi>n</mml:mi><mml:mo>â^'</mml:mo><mml:mn>1</mml:m phases studied using density functional theory. Physical Review B, 2014, 90, .	3.2	33
25	Vacancy-mediated diffusion in disordered alloys: Ge self-diffusion inSi1â^'xGex. Physical Review B, 2002, 65, .	3.2	32
26	Hole-Mediated Stabilization of Cubic GaN. Physical Review Letters, 2004, 93, 216401.	7.8	32
27	Symmetry Considerations in CdSe Nanocrystals. Nano Letters, 2006, 6, 501-504.	9.1	31
28	Oxidation of free-standing and supported borophene. 2D Materials, 2017, 4, 025025.	4.4	31
29	Realization of predicted exotic materials: The burden of proof. Materials Today, 2020, 32, 35-45.	14.2	29
30	Dalpian and Chelikowsky Reply:. Physical Review Letters, 2008, 100, .	7.8	28
31	Antidoping in Insulators and Semiconductors Having Intermediate Bands with Trapped Carriers. Physical Review Letters, 2019, 122, 106403.	7.8	28
32	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
33	Role of Confinement on Diffusion Barriers in Semiconductor Nanocrystals. Physical Review Letters, 2009, 102, 025901.	7.8	27
34	Ferrimagnetic Fe-doped GaN: An unusual magnetic phase in dilute magnetic semiconductors. Physical Review B, 2009, 79, .	3.2	27
35	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
36	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

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37	First-principles study of Mn-induced local magnetic moments in host semiconductors. Physical Review B, 2005, 71, .	3.2	23
38	Electron-mediated ferromagnetism and negativesâˆ’dexchange splitting in semiconductors. Physical Review B, 2006, 73, .	3.2	23
39	High temperature activation of hematite nanorods for sunlight driven water oxidation reaction. Physical Chemistry Chemical Physics, 2017, 19, 25025-25032.	2.8	23
40	Zeeman-type spin splitting in nonmagnetic three-dimensional compounds. Npj Quantum Materials, 2019, 4, .	5.2	23
41	Different shapes of spin textures as a journey through the Brillouin zone. Physical Review B, 2021, 104, .	3.2	23
42	Effect of Charges on the Interaction of a Water Molecule with the Fe₂O₃(0001) Surface. Journal of Physical Chemistry C, 2016, 120, 11918-11925.	3.1	22
43	First-principles calculations of lattice-strained core-shell nanocrystals. Physical Review B, 2011, 84, .	3.2	21
44	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
45	Impurity-induced phase stabilization of semiconductors. Applied Physics Letters, 2006, 89, 011907.	3.3	20
46	Inverse design of compounds that have simultaneously ferroelectric and Rashba cofunctionality. Physical Review B, 2020, 102, .	3.2	20
47	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
48	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
49	Transition from ferromagnetism to antiferromagnetism in Ga1âˆ’xMnxN. Journal of Applied Physics, 2005, 98, 083905.	2.5	18
50	Quantum confinement effects on Mn-doped InAs nanocrystals: A first-principles study. Physical Review B, 2008, 78, .	3.2	18
51	First principles investigations on the electronic structure of anchor groups on ZnO nanowires and surfaces. Journal of Applied Physics, 2014, 115, .	2.5	16
52	<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>Simulation 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
53	Ab initio calculations of vacancies in SixGe1âˆ’x. Applied Physics Letters, 2002, 81, 3383-3385.	3.3	14
54	Photoinduced cation interstitial diffusion in IIâ€“VI semiconductors. Physical Review B, 2005, 72, .	3.2	14

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55	Liquid separation by a graphene membrane. Journal of Applied Physics, 2010, 108, 113527.	2.5	14
56	Oxygen vacancies at the surface of SrTiO₃ thin films. Journal of Applied Physics, 2014, 115, 033710.	2.5	14
57	MXene Phase with C₃ Structure Unit: A Family of 2D Electrides. Advanced Functional Materials, 2021, 31, 2100009.	14.9	13
58	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
59	Cobalt-doped ZnO nanocrystals: quantum confinement and surface effects from ab initio methods. Physical Chemistry Chemical Physics, 2013, 15, 15863.	2.8	12
60	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
61	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
62	Computational screening of bulk materials with intrinsic intermediate band. Computational Materials Science, 2019, 158, 382-388.	3.0	10
63	Intrinsic doping limitations in inorganic lead halide perovskites. Materials Horizons, 2022, 9, 791-803.	12.2	10
64	Adsorption of Mn atoms on the Si(100) surface. Surface Science, 2004, 566-568, 688-692.	1.9	9
65	Evidence for a subtle structural symmetry breaking in EuB₆. Journal of Physics Condensed Matter, 2009, 21, 456007.	1.8	9
66	Emergence of competing magnetic interactions induced by Ge doping in the semiconductorFeGa3. Physical Review B, 2016, 94, .	3.2	9
67	Tailoring the Optical, Electronic, and Magnetic Properties of MAPbI₃ through Self-Assembled Fe Incorporation. Journal of Physical Chemistry C, 2021, 125, 15636-15646.	3.1	9
68	Adsorption of monomers on semiconductors and the importance of surface degrees of freedom. Physical Review B, 2001, 63, .	3.2	8
69	Carrier-induced enhancement and suppression of ferromagnetism in Zn_{1-x}Cr_xTe and Ga_{1-x}Cr_xAs: origin of the spinodal decomposition. New Journal of Physics, 2008, 10, 113007.	2.9	8
70	Vacancies at LaAlO3 thin films: A 2D electron gas at the surface. Journal of Alloys and Compounds, 2016, 684, 544-548.	5.5	8
71	Semiclassical transport properties of IrGa₃: a promising thermoelectric material. Journal of Physics Condensed Matter, 2018, 30, 085701.	1.8	7
72	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

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73	Band coupling model of electron and hole mediated ferromagnetism in semiconductors: the case of GaN. , 2008, , .		6
74	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
75	Two-Atom Structures of Ge on Si(100): Dimers versus Adatom Pairs. Physical Review Letters, 2001, 87, 036104.	7.8	5
76	Surface-induced structural modification in ZnO nanoparticles. Journal of Nanoparticle Research, 2012, 14, 1.	1.9	5
77	Conduction electron spin resonance in AlB₂. Journal of Physics Condensed Matter, 2013, 25, 216001.	1.8	5
78	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:mi><mml:m Physical Review B, 2020, 102, .		5
79	Insulatorâ€“Metal Transition in the Nd₂CoFeO₆ Disordered Double Perovskite. Journal of Physical Chemistry C, 2020, 124, 22733-22742.	3.1	5
80	Possible Charge-Transfer-Induced Conductivity Enhancement in TiO₂ Microtubes Decorated with Perovskite CsPbBr₃ Nanocrystals. Langmuir, 2020, 36, 5408-5416.	3.5	5
81	Tuning hydrogen adsorption and electronic properties from graphene to fluorographone. Physical Review Materials, 2020, 4, .	2.4	5
82	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
83	Initial stages of Ge and Si growth nearSBmonoatomic steps on Si(100). Physical Review B, 2004, 70, .	3.2	3
84	Preface to the Forum on Materials Discovery and Design. ACS Applied Materials & Interfaces, 2019, 11, 24823-24824.	8.0	3
85	Impurity-stabilized zinc-blende phase of wurtzite compounds. Journal of Physics and Chemistry of Solids, 2005, 66, 2008-2010.	4.0	2
86	A systematic first-principles study of the tungsten trioxide polymorphs. Physica Status Solidi (B): Basic Research, 2015, 252, 2290-2295.	1.5	2
87	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
88	High-throughput inverse design and Bayesian optimization of functionalities: spin splitting in two-dimensional compounds. Scientific Data, 2022, 9, 195.	5.3	2
89	Electronic mechanism for resistive switching in metal/insulator/metal nanodevices. Journal Physics D: Applied Physics, 2020, 53, 295302.	2.8	1
90	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

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91	Theoretical STM images of Ge monomers and trimers on Si(100). Surface Science, 2001, 482-485, 507-511.	1.9	0
92	Stabilization of Zinc-Blende Semiconductors Through 3d Impurities and Holes. AIP Conference Proceedings, 2005, , .	0.4	0
93	Spins in Semiconductor Nanocrystals. , 2018, , 1-12.		0
94	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
95	Spins in Semiconductor Nanocrystals. , 2020, , 605-616.		0
96	Pressure-Induced Stabilization of Sodium Halide Perovskites. Journal of Physical Chemistry C, 2022, 126, 4248-4254.	3.1	0