Eduardo Menendez Proupin

List of Publications by Year
in descending order

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73 papers	1,594 citations	361413 20 h-index	315739 38 g-index
75 all docs	75 docs citations	75 times ranked	2564 citing authors

#	Article	IF	Citations
1	Mixed-anion mixed-cation perovskite (FAPbI₃)_{0.875}(MAPbBr₃)_{0.125}: an ab initio molecular dynamics study. Journal of Materials Chemistry A, 2022, 10, 9592-9603.	10.3	4
2	Phenomenological model for long-wavelength optical modes in transition metal dichalcogenide monolayer. Physical Review B, 2021, 103, .	3.2	5
3	Chemical Diversity in Lead-Free, Layered Double Perovskites: A Combined Experimental and Computational Approach. Chemistry of Materials, 2020, 32, 424-429.	6.7	52
4	Inducing a level inside of CdTe bandgap doping with Sn using a co-sublimation technique by CSS. Materials Science in Semiconductor Processing, 2020, 107, 104836.	4.0	2
5	Methodological Issues in First-Principle Calculations of CH₃NH₃PbI₃ Perovskite Surfaces: Quantum Confinement and Thermal Motion. ACS Omega, 2020, 5, 29477-29491.	3.5	9
6	Atomic-Scale Model and Electronic Structure of Cu2O/CH3NH3PbI3 Interfaces in Perovskite Solar Cells. ACS Applied Materials & Interfaces, 2020, 12, 44648-44657.	8.0	16
7	Bismuth Doping of CdTe: The Effect of Spinâ€“Orbit Coupling. Physica Status Solidi (B): Basic Research, 2020, 257, 1900693.	1.5	0
8	Self-compensation in chlorine-doped CdTe. Scientific Reports, 2019, 9, 9194.	3.3	13
9	Symmetry and thermodynamics of tellurium vacancies in cadmium telluride. Physica B: Condensed Matter, 2019, 568, 81-87.	2.7	1
10	Energetics and Electronic Properties of Interstitial Chlorine in CdTe. Physica Status Solidi (B): Basic Research, 2019, 256, 1800219.	1.5	4
11	Electronic and thermal properties of non-stoichiometric and doped cobaltum antimonide. Materials Research Express, 2018, 5, 025908.	1.6	3
12	Influence of chromium hyperdoping on the electronic structure of CH3NH3PbI3 perovskite: a first-principles insight. Scientific Reports, 2018, 8, 2511.	3.3	13
13	Density functional theory study of defects in cadmium telluride: a PBC and QM/MM comparison. Journal of Physics: Conference Series, 2018, 1043, 012043.	0.4	0
14	Accuracy of the Heyd-Scuseria-Ernzerhof hybrid functional to describe many-electron interactions and charge localization in semiconductors. Physical Review B, 2018, 98, .	3.2	13
15	Theoretical study of bismuth-doped CdTe. Journal of Physics: Conference Series, 2018, 1043, 012044.	0.4	1
16	Optical, Electronic, and Magnetic Engineering of âŸ¨111âŸ© Layered Halide Perovskites. Chemistry of Materials, 2018, 30, 5315-5321.	6.7	69
17	Sn-doped CdTe as promising intermediate-band photovoltaic material. Journal Physics D: Applied Physics, 2017, 50, 035501.	2.8	17
18	Self-compensation in phosphorus-doped CdTe. Physical Review B, 2017, 96, .	3.2	13

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19	Ferroelectric Domains May Lead to Two-Dimensional Confinement of Holes, but not of Electrons, in CH₃NH₃PbI₃ Perovskite. Journal of Physical Chemistry C, 2017, 121, 26698-26705.	3.1	11
20	First principle study of V-implantation in highly-doped silicon materials. Computational Materials Science, 2017, 136, 207-215.	3.0	6
21	Theoretical study of intrinsic defects in CdTe. Journal of Physics: Conference Series, 2016, 720, 012031.	0.4	5
22	Sn doped CdTe as candidate for intermediate-band solar cells: A first principles DFT+GW study. Journal of Physics: Conference Series, 2016, 720, 012033.	0.4	1
23	Spin-orbit coupling effects in gold clusters: The case of Au₁₃. Journal of Physics: Conference Series, 2016, 720, 012034.	0.4	6
24	Modeling of Thermal Effect on the Electronic Properties of Photovoltaic Perovskite CH₃NH₃PbI₃: The Case of Tetragonal Phase. Journal of Physical Chemistry C, 2016, 120, 7976-7986.	3.1	25
25	First-principles DFT +GW study of the Te antisite in CdTe. Computational Materials Science, 2016, 125, 176-182.	3.0	12
26	First-principles<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>G</mml:mi> of oxygen-doped CdTe. Physical Review B, 2016, 93, .	3.2	9
27	Tellurium vacancy in cadmium telluride revisited: Size effects in the electronic properties. Physica Status Solidi (B): Basic Research, 2015, 252, 2649-2656.	1.5	11
28	Nonhydrogenic exciton spectrum in perovskite CH₃NH₃PbI₃. Physica Status Solidi - Rapid Research Letters, 2015, 9, 559-563.	2.4	34
29	Evolution of the doping regimes in the Al-doped SnO₂nanoparticles prepared by a polymer precursor method. Journal of Physics Condensed Matter, 2015, 27, 095301.	1.8	44
30	Electronic and atomic structure of complex defects in Al- and Ga-highly doped ZnO films. Materials Chemistry and Physics, 2015, 160, 420-428.	4.0	8
31	Elastic constants and Debye temperature of wz-AlN and wz-GaN semiconductors under high pressure from first-principles. Pramana - Journal of Physics, 2014, 83, 413-425.	1.8	7
32	The absorption spectrum of C60 in n-hexane solution revisited: Fitted experiment and TDDFT/PCM calculations. Chemical Physics Letters, 2014, 593, 72-76.	2.6	14
33	Electronic structure of CdTe using GGA+USIC. Physica B: Condensed Matter, 2014, 452, 119-123.	2.7	21
34	Self-consistent relativistic band structure of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">CH</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">NH</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">PbI</mml:mi><mml:msub><mml:mr	3.2	245
35	Paramagnetic shift in thermally annealed CdxZn1â^'xSe quantum dots. New Journal of Physics, 2012, 14, 043038.	2.9	11
36	Electronic excitations of C60 aggregates. Physical Chemistry Chemical Physics, 2012, 14, 13058.	2.8	15

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37	Ultrathin Carbon Nanotube With Single, Double, and Triple Bonds. Physical Review Letters, 2012, 109, 105501.	7.8	8
38	Nitrogen/gold codoping of the TiO2(101) anatase surface. A theoretical study based on DFT calculations. Physical Chemistry Chemical Physics, 2011, 13, 11340.	2.8	38
39	Computer simulation of elastic constants of hydroxyapatite and fluorapatite. Journal of the Mechanical Behavior of Biomedical Materials, 2011, 4, 1011-1020.	3.1	68
40	Core-level shift analysis of amorphous CdTeO x materials. Journal of Materials Science, 2010, 45, 5071-5076.	3.7	6
41	Atomistic study of vibrational properties of Î³-Al2O3. Journal of Materials Science, 2010, 45, 5094-5100.	3.7	22
42	Computer simulation study of amorphous compounds: structural and vibrational properties. Journal of Materials Science, 2010, 45, 5124-5134.	3.7	14
43	Characterization of spin-state tuning in thermally annealed semiconductor quantum dots. Physical Review B, 2010, 82, .	3.2	12
44	Quantitative local environment characterization in amorphous oxides. Physical Review B, 2010, 81, .	3.2	16
45	Approximate quantum mechanical method for describing excitations and related properties of finite single-walled carbon nanotubes. Physical Review B, 2010, 81, .	3.2	9
46	Ab initiomolecular dynamics study of amorphousCdTeOxalloys: Structural properties. Physical Review B, 2009, 79, .	3.2	8
47	Strength of polycrystalline coarse-grained platinum to 330GPa and of nanocrystalline platinum to 70GPa from high-pressure x-ray diffraction data. Journal of Applied Physics, 2008, 103, .	2.5	22
48	Ab initiocalculations of elastic properties of compressed Pt. Physical Review B, 2007, 76, .	3.2	35
49	Nonhydrostatic compression of bismuth to 222GPa: Some constraints on elasticity of the bcc-phase. Journal of Physics and Chemistry of Solids, 2006, 67, 2192-2196.	4.0	6
50	Ab initio study of Ti3Si0.5Ge0.5C2 under pressure. Journal of Physics and Chemistry of Solids, 2006, 67, 2149-2153.	4.0	5
51	Excitonâ€“phonon complexes and optical properties in CdSe nanocrystals. Journal of Physics Condensed Matter, 2006, 18, 7283-7298.	1.8	0
52	Proposal for a modified MÃ¸ller-Plesset perturbation theory. Physical Review A, 2006, 73, .	2.5	3
53	Elastic properties of the bcc structure of bismuth at high pressure. Journal of Applied Physics, 2006, 99, 103504.	2.5	28
54	Publisher's Note: Electronic properties of bulkÎ³â€²Al2O3 [Phys. Rev. B72, 035116 (2005)]. Physical Review B, 2005, 72, .	3.2	3

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55	Electronic properties of bulkÎ³â^'Al2O3. Physical Review B, 2005, 72, .	3.2	103
56	Electronic structure of crystalline binary and ternaryCdâ^'Teâ^'Ocompounds. Physical Review B, 2004, 70, .	3.2	37
57	Electric-field and exciton structure in CdSe nanocrystals. Physical Review B, 2004, 69, .	3.2	36
58	Comment on â€œThe effects of electric field on the electronic structure of a semiconductor quantum dotâ€•[J. Appl. Phys.84, 1454 (1998)]. Journal of Applied Physics, 2004, 95, 3223-3224.	2.5	1
59	Stark effect in CdSe nanocrystals. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, S42-S45.	0.8	1
60	Electronic structure of binary and ternary components of CdTe:O thin films. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, S104-S107.	0.8	6
61	Resonant Raman scattering off neutral quantum dots. Physical Review B, 2002, 65, .	3.2	6
62	Resonance Raman scattering in semiconductor quantum dots: Adiabatic versus time-dependent perturbation theory. Physical Review B, 2002, 66, .	3.2	6
63	COMPOSITION MIXTURE PROBABILISTIC MODEL IN THE FORMATION OF SEMICONDUCTOR MATERIALS OBTAINED BY RANDOM GROWTH TECHNIQUES. Modern Physics Letters B, 2001, 15, 643-646.	1.9	6
64	Interband absorption and luminescence in small quantum dots under strong magnetic fields. Physica E: Low-Dimensional Systems and Nanostructures, 2000, 8, 333-341.	2.7	2
65	Multiphonon resonant Raman scattering in nanocrystals. Physical Review B, 2000, 62, 11006-11016.	3.2	42
66	Resonant hyper-Raman scattering in spherical quantum dots. Physical Review B, 1999, 60, 5513-5522.	3.2	14
67	Experimental evidence of compositional mixture in CdTeO films grown by radio-frequency sputtering. Journal of Applied Physics, 1999, 86, 4688-4690.	2.5	19
68	Resonant Raman scattering in self-assembled quantum dots. Physical Review B, 1999, 60, 16747-16757.	3.2	22
69	Resonant Raman Scattering in Asymmetric Semiconductor Quantum Disks. Physica Status Solidi (B): Basic Research, 1999, 215, 459-463.	1.5	2
70	Exciton and confinement potential effects on the resonant Raman scattering in quantum dots. Semiconductor Science and Technology, 1998, 13, 871-875.	2.0	6
71	Optical vibrons in CdSe dots and dispersion relation of the bulk material. Physical Review B, 1998, 57, 4664-4669.	3.2	213
72	Vibrational Resonant Raman Scattering in Spherical Quantum Dots: Exciton Effects. Physica Status Solidi (B): Basic Research, 1997, 199, 81-94.	1.5	46

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73	Impurity absorption in spherical quantum dots. AIP Conference Proceedings, 1996, , .	0.4	0