# 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 | 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:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math> perovskite. | 3.2 | 245 |
| 2 | Optical vibrons in CdSe dots and dispersion relation of the bulk material. Physical Review B, 1998, 57, 4664-4669. | 3.2 | 213 |
| 3 | Electronic properties of bulkÎ³â^'Al2O3. Physical Review B, 2005, 72, . | 3.2 | 103 |
| 4 | Optical, Electronic, and Magnetic Engineering of âŸ¨111âŸ© Layered Halide Perovskites. Chemistry of Materials, 2018, 30, 5315-5321. | 6.7 | 69 |
| 5 | Computer simulation of elastic constants of hydroxyapatite and fluorapatite. Journal of the Mechanical Behavior of Biomedical Materials, 2011, 4, 1011-1020. | 3.1 | 68 |
| 6 | Chemical Diversity in Lead-Free, Layered Double Perovskites: A Combined Experimental and Computational Approach. Chemistry of Materials, 2020, 32, 424-429. | 6.7 | 52 |
| 7 | Vibrational Resonant Raman Scattering in Spherical Quantum Dots: Exciton Effects. Physica Status Solidi (B): Basic Research, 1997, 199, 81-94. | 1.5 | 46 |
| 8 | Evolution of the doping regimes in the Al-doped SnO<sub>2</sub>nanoparticles prepared by a polymer precursor method. Journal of Physics Condensed Matter, 2015, 27, 095301. | 1.8 | 44 |
| 9 | Multiphonon resonant Raman scattering in nanocrystals. Physical Review B, 2000, 62, 11006-11016. | 3.2 | 42 |
| 10 | 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 |
| 11 | Electronic structure of crystalline binary and ternaryCdâ^'Teâ^'Ocompounds. Physical Review B, 2004, 70, . | 3.2 | 37 |
| 12 | Electric-field and exciton structure in CdSe nanocrystals. Physical Review B, 2004, 69, . | 3.2 | 36 |
| 13 | Ab initiocalculations of elastic properties of compressed Pt. Physical Review B, 2007, 76, . | 3.2 | 35 |
| 14 | Nonhydrogenic exciton spectrum in perovskite CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>. Physica Status Solidi - Rapid Research Letters, 2015, 9, 559-563. | 2.4 | 34 |
| 15 | Elastic properties of the bcc structure of bismuth at high pressure. Journal of Applied Physics, 2006, 99, 103504. | 2.5 | 28 |
| 16 | Modeling of Thermal Effect on the Electronic Properties of Photovoltaic Perovskite CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>: The Case of Tetragonal Phase. Journal of Physical Chemistry C, 2016, 120, 7976-7986. | 3.1 | 25 |
| 17 | Resonant Raman scattering in self-assembled quantum dots. Physical Review B, 1999, 60, 16747-16757. | 3.2 | 22 |
| 18 | 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 |

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|---|---|---|---|
| 19 | Atomistic study of vibrational properties of Î³-Al2O3. Journal of Materials Science, 2010, 45, 5094-5100. | 3.7 | 22 |
| 20 | Electronic structure of CdTe using GGA+USIC. Physica B: Condensed Matter, 2014, 452, 119-123. | 2.7 | 21 |
| 21 | Experimental evidence of compositional mixture in CdTeO films grown by radio-frequency sputtering. Journal of Applied Physics, 1999, 86, 4688-4690. | 2.5 | 19 |
| 22 | Sn-doped CdTe as promising intermediate-band photovoltaic material. Journal Physics D: Applied Physics, 2017, 50, 035501. | 2.8 | 17 |
| 23 | Quantitative local environment characterization in amorphous oxides. Physical Review B, 2010, 81, . | 3.2 | 16 |
| 24 | 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 |
| 25 | Electronic excitations of C60 aggregates. Physical Chemistry Chemical Physics, 2012, 14, 13058. | 2.8 | 15 |
| 26 | Resonant hyper-Raman scattering in spherical quantum dots. Physical Review B, 1999, 60, 5513-5522. | 3.2 | 14 |
| 27 | Computer simulation study of amorphous compounds: structural and vibrational properties. Journal of Materials Science, 2010, 45, 5124-5134. | 3.7 | 14 |
| 28 | 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 |
| 29 | Self-compensation in phosphorus-doped CdTe. Physical Review B, 2017, 96, . | 3.2 | 13 |
| 30 | Influence of chromium hyperdoping on the electronic structure of CH3NH3PbI3 perovskite: a first-principles insight. Scientific Reports, 2018, 8, 2511. | 3.3 | 13 |
| 31 | 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 |
| 32 | Self-compensation in chlorine-doped CdTe. Scientific Reports, 2019, 9, 9194. | 3.3 | 13 |
| 33 | Characterization of spin-state tuning in thermally annealed semiconductor quantum dots. Physical Review B, 2010, 82, . | 3.2 | 12 |
| 34 | First-principles DFT +GW study of the Te antisite in CdTe. Computational Materials Science, 2016, 125, 176-182. | 3.0 | 12 |
| 35 | Paramagnetic shift in thermally annealed CdxZn1â^'xSe quantum dots. New Journal of Physics, 2012, 14, 043038. | 2.9 | 11 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Ferroelectric Domains May Lead to Two-Dimensional Confinement of Holes, but not of Electrons, in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> Perovskite. Journal of Physical Chemistry C, 2017, 121, 26698-26705. | 3.1 | 11 |
| 38 | Approximate quantum mechanical method for describing excitations and related properties of finite single-walled carbon nanotubes. Physical Review B, 2010, 81, . | 3.2 | 9 |
| 39 | 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 |
| 40 | Methodological Issues in First-Principle Calculations of CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> Perovskite Surfaces: Quantum Confinement and Thermal Motion. ACS Omega, 2020, 5, 29477-29491. | 3.5 | 9 |
| 41 | Ab initiomolecular dynamics study of amorphousCdTeOxalloys: Structural properties. Physical Review B, 2009, 79, . | 3.2 | 8 |
| 42 | Ultrathin Carbon Nanotube With Single, Double, and Triple Bonds. Physical Review Letters, 2012, 109, 105501. | 7.8 | 8 |
| 43 | 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 |
| 44 | 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 |
| 45 | Exciton and confinement potential effects on the resonant Raman scattering in quantum dots. Semiconductor Science and Technology, 1998, 13, 871-875. | 2.0 | 6 |
| 46 | 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 |
| 47 | Resonant Raman scattering off neutral quantum dots. Physical Review B, 2002, 65, . | 3.2 | 6 |
| 48 | Resonance Raman scattering in semiconductor quantum dots: Adiabatic versus time-dependent perturbation theory. Physical Review B, 2002, 66, . | 3.2 | 6 |
| 49 | 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 |
| 50 | 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 |
| 51 | Core-level shift analysis of amorphous CdTeO x materials. Journal of Materials Science, 2010, 45, 5071-5076. | 3.7 | 6 |
| 52 | Spin-orbit coupling effects in gold clusters: The case of Au<sub>13</sub>. Journal of Physics: Conference Series, 2016, 720, 012034. | 0.4 | 6 |
| 53 | First principle study of V-implantation in highly-doped silicon materials. Computational Materials Science, 2017, 136, 207-215. | 3.0 | 6 |
| 54 | Ab initio study of Ti3Si0.5Ge0.5C2 under pressure. Journal of Physics and Chemistry of Solids, 2006, 67, 2149-2153. | 4.0 | 5 |

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|---|---|---|---|
| 55 | Theoretical study of intrinsic defects in CdTe. Journal of Physics: Conference Series, 2016, 720, 012031. | 0.4 | 5 |
| 56 | Phenomenological model for long-wavelength optical modes in transition metal dichalcogenide monolayer. Physical Review B, 2021, 103, . | 3.2 | 5 |
| 57 | Energetics and Electronic Properties of Interstitial Chlorine in CdTe. Physica Status Solidi (B): Basic Research, 2019, 256, 1800219. | 1.5 | 4 |
| 58 | Mixed-anion mixed-cation perovskite (FAPbI<sub>3</sub>)<sub>0.875</sub>(MAPbBr<sub>3</sub>)<sub>0.125</sub>: an ab initio molecular dynamics study. Journal of Materials Chemistry A, 2022, 10, 9592-9603. | 10.3 | 4 |
| 59 | Publisher's Note: Electronic properties of bulkÎ³â^'Al2O3 [Phys. Rev. B72, 035116 (2005)]. Physical Review B, 2005, 72, . | 3.2 | 3 |
| 60 | Proposal for a modified MÃ¸ller-Plesset perturbation theory. Physical Review A, 2006, 73, . | 2.5 | 3 |
| 61 | Electronic and thermal properties of non-stoichiometric and doped cobaltum antimonide. Materials Research Express, 2018, 5, 025908. | 1.6 | 3 |
| 62 | Resonant Raman Scattering in Asymmetric Semiconductor Quantum Disks. Physica Status Solidi (B): Basic Research, 1999, 215, 459-463. | 1.5 | 2 |
| 63 | 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 |
| 64 | 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 |
| 65 | 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 |
| 66 | Stark effect in CdSe nanocrystals. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, S42-S45. | 0.8 | 1 |
| 67 | 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 |
| 68 | Theoretical study of bismuth-doped CdTe. Journal of Physics: Conference Series, 2018, 1043, 012044. | 0.4 | 1 |
| 69 | Symmetry and thermodynamics of tellurium vacancies in cadmium telluride. Physica B: Condensed Matter, 2019, 568, 81-87. | 2.7 | 1 |
| 70 | Impurity absorption in spherical quantum dots. AIP Conference Proceedings, 1996, , . | 0.4 | 0 |
| 71 | Excitonâ€“phonon complexes and optical properties in CdSe nanocrystals. Journal of Physics Condensed Matter, 2006, 18, 7283-7298. | 1.8 | 0 |
| 72 | 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 |

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|---|---|---|---|
| 73 | Bismuth Doping of CdTe: The Effect of Spinâ€“Orbit Coupling. Physica Status Solidi (B): Basic Research, 2020, 257, 1900693. | 1.5 | 0 |