Pablo Palacios

List of Publications by Year
in descending order

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62	1,901	257450 24	254184 43
papers	citations	h-index	g-index

63	63	63	2062
all docs	docs citations	times ranked	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 />	3.2	245
2	Transition-Metal-Substituted Indium Thiospinels as Novel Intermediate-Band Materials: Prediction and Understanding of Their Electronic Properties. Physical Review Letters, 2008, 101, 046403.	7.8	129
3	Theoretical modelling of intermediate band solar cell materials based on metal-doped chalcopyrite compounds. Thin Solid Films, 2007, 515, 6280-6284.	1.8	96
4	Synthesis and Spectral Properties of Nanocrystalline V-Substituted In2S3, a Novel Material for More Efficient Use of Solar Radiation. Chemistry of Materials, 2008, 20, 5125-5127.	6.7	95
5	Formation of a reliable intermediate band in Si heavily coimplanted with chalcogens (S, Se, Te) and group III elements (B, Al). Physical Review B, 2010, 82, .	3.2	83
6	Assessment through first-principles calculations of an intermediate-band photovoltaic material based on Ti-implanted silicon: Interstitial versus substitutional origin. Physical Review B, 2009, 79, .	3.2	81
7	V-doped SnS2: a new intermediate band material for a better use of the solar spectrum. Physical Chemistry Chemical Physics, 2011, 13, 20401.	2.8	80
8	First principles calculation of isolated intermediate bands formation in a transition metal-doped chalcopyrite-type semiconductor. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 1395-1401.	1.8	77
9	Solution-based synthesis and processing of Sn- and Bi-doped Cu₃SbSe₄nanocrystals, nanomaterials and ring-shaped thermoelectric generators. Journal of Materials Chemistry A, 2017, 5, 2592-2602.	10.3	73
10	First-principles investigation of isolated band formation in half-metallicTixGa1â^'xP(x=0.3125â€“0.25). Physical Review B, 2006, 73, .	3.2	56
11	Thermodynamics of the Formation of Ti- and Cr-doped CuGaS₂ Intermediate-band Photovoltaic Materials. Journal of Physical Chemistry C, 2008, 112, 9525-9529.	3.1	50
12	Enhancement of optical absorption in Ga-chalcopyrite-based intermediate-band materials for high efficiency solar cells. Solar Energy Materials and Solar Cells, 2010, 94, 1903-1906.	6.2	48
13	Energetics of formation of TiGa3As4 and TiGa3P4 intermediate band materials. Journal of Chemical Physics, 2006, 124, 014711.	3.0	47
14	Optical properties of chalcopyrite-type intermediate transition metal band materials from first principles. Thin Solid Films, 2008, 516, 7055-7059.	1.8	47
15	Theoretical optoelectronic analysis of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgIn</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml	3.2	45
16	V-substituted In₂S₃: an intermediate band material with photocatalytic activity in the whole visible light range. Journal of Materials Chemistry A, 2014, 2, 8236-8245.	10.3	42
17	Ab-initio valence band spectra of Al, In doped ZnO. Thin Solid Films, 2009, 517, 2448-2451.	1.8	41
18	Thermoelectric Properties of Doped-Cu₃SbSe₄ Compounds: A First-Principles Insight. Inorganic Chemistry, 2018, 57, 7321-7333.	4.0	36

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19	Effect of van der Waals interaction on the properties of SnS2 layered semiconductor. Thin Solid Films, 2013, 535, 387-389.	1.8	33
20	Band gap control via tuning of inversion degree in CdIn2S4 spinel. Applied Physics Letters, 2012, 100, .	3.3	31
21	Tetrabutylammonium (TBA)-Doped Methylammonium Lead Iodide: High Quality and Stable Perovskite Thin Films. Frontiers in Energy Research, 2022, 10, .	2.3	30
22	Electronic structure and optical properties in ZnO:M(Co, Cd). Thin Solid Films, 2010, 518, 4568-4571.	1.8	26
23	First principles characterization of direct transitions for high efficiency new photovoltaic materials. Computational Materials Science, 2003, 27, 58-64.	3.0	25
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	Ab-initio spin polarized electronic structure calculations for TixGanAsm photovoltaic materials. Journal of Materials Science, 2005, 40, 1383-1386.	3.7	24
26	Electronic structure of bulk- and Na-intercalated<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiS</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu from a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>GGA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> with the Hubbard terms obtainedab initio. Physical Review B, 2008, 78, .	3.2	24
27	Characterization by Ab Initio Calculations of an Intermediate Band Material Based on Chalcopyrite Semiconductors Substituted by Several Transition Metals. Journal of Solar Energy Engineering, Transactions of the ASME, 2007, 129, 314.	1.8	22
28	Intermediate band position modulated by Zn addition in Ti doped CuGaS2. Thin Solid Films, 2011, 519, 7517-7521.	1.8	20
29	Obtaining an intermediate band photovoltaic material through the Bi insertion in CdTe. Solar Energy Materials and Solar Cells, 2013, 114, 99-103.	6.2	18
30	Properties of intermediate band materials. Solar Energy Materials and Solar Cells, 2005, 87, 323-331.	6.2	17
31	Ab-initio vibrational properties of transition metal chalcopyrite alloys determined as high-efficiency intermediate-band photovoltaic materials. Thin Solid Films, 2008, 516, 7070-7074.	1.8	16
32	Screened hybrid and self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="italic">GW</mml:mi></mml:mrow></mml:math>calculations of cadmium/magnesium indium sulfide materials. Physical Review B, 2011, 83, .	3.2	16
33	Electronic band alignment at CuGaS2 chalcopyrite interfaces. Computational Materials Science, 2016, 121, 79-85.	3.0	16
34	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
35	Theoretical band alignment in an intermediate band chalcopyrite based material. Applied Surface Science, 2017, 424, 132-136.	6.1	15
36	Understanding Ti intermediate-band formation in partially inverse thiospinel MgIn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>S<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>through many-body approaches. Physical Review B, 2011, 84, .	3.2	14

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37	Influence of chromium hyperdoping on the electronic structure of CH3NH3PbI3 perovskite: a first-principles insight. Scientific Reports, 2018, 8, 2511.	3.3	13
38	Ab initio phonon dispersion calculations for TixGanAsm and TixGanPm compounds. Computational Materials Science, 2005, 33, 118-124.	3.0	12
39	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
40	Thermodynamics of zinc insertion in CuGaS2:Ti, used as a modulator agent in an intermediate-band photovoltaic material. Computational and Theoretical Chemistry, 2011, 975, 134-137.	2.5	10
41	Vanadium supersaturated silicon system: a theoretical and experimental approach. Journal Physics D: Applied Physics, 2017, 50, 495101.	2.8	10
42	Characterization of electrodeposited zinc oxide/tetrasulphonatedcopper phthalocyanines (ZnO/Ts-CuPc) hybrid films and their photoelectrochemical properties. Journal of Electroanalytical Chemistry, 2011, 653, 86-92.	3.8	9
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	Transition Metal-Hyperdoped InP Semiconductors as Efficient Solar Absorber Materials. Nanomaterials, 2020, 10, 283.	4.1	8
45	Spinel-Type nitride compounds with improved features as solar cell absorbers. Acta Materialia, 2020, 197, 316-329.	7.9	7
46	The effects of the chemical composition on the structural, thermodynamic, and mechanical properties of all-inorganic halide perovskites. Inorganic Chemistry Frontiers, 2021, 8, 3803-3814.	6.0	7
47	First principle study of V-implantation in highly-doped silicon materials. Computational Materials Science, 2017, 136, 207-215.	3.0	6
48	Active Materials Based on Implanted Si for Obtaining Intermediate Band Solar Cells. Advances in Science and Technology, 0, , .	0.2	5
49	Double Ion Implantation and Pulsed Laser Melting Processes for Third Generation Solar Cells. International Journal of Photoenergy, 2013, 2013, 1-7.	2.5	5
50	Analysis of SnS₂hyperdoped with V proposed as efficient absorber material. Journal of Physics Condensed Matter, 2014, 26, 395501.	1.8	5
51	Band Alignment of the CuGaS2 Chalcopyrite Interfaces Studied by First-Principles Calculations. ACS Omega, 2020, 5, 3294-3301.	3.5	5
52	Progress towards the practical implementation of the intermediate band solar cell. , 0, , .		4
53	Tight-binding electronic band structure and surface states of Cu-chalcopyrite semiconductors. Journal of Physics Communications, 2018, 2, 035021.	1.2	4
54	Thermoradiative Cells Based on a p-type Cu3SbSe4 Semiconductor: Application of a Detailed Balance Model. Journal of Electronic Materials, 2019, 48, 6777-6785.	2.2	4

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55	Atomistic Simulation of the Equation of State of SrF 2 Using Electron Gas Interionic Potentials. High Pressure Research, 2002, 22, 227-230.	1.2	3
56	Cation substitution effects on the structural, electronic and sun-light absorption features of all-inorganic halide perovskites. Inorganic Chemistry Frontiers, 2022, 9, 1337-1353.	6.0	2
57	AB-Initio Modeling of Intermediate Band Materials Based on Metal-Doped Chalcopyrite Compounds. , 2006, , .		1
58	Advanced Computational Design of Intermediate-Band Photovoltaic Material V-substituted MgIn2S4. Materials Research Society Symposia Proceedings, 2009, 1218, 1.	0.1	1
59	Towards an ab-initio characterization of novel intermediate band photovoltaic materials. Optoelectronic and Microelectronic Materials and Devices (COMMAD), Conference on, 2008, , .	0.0	0
60	First Principles Calculations of Complex Intermediate Band Materials for Photovoltaic Devices. Materials Research Society Symposia Proceedings, 2009, 1211, 1.	0.1	0
61	DiseÃ±o de nuevos materiales fotovoltaicos de banda intermedia. Boletin De La Sociedad Espanola De Ceramica Y Vidrio, 2004, 43, 345-347.	1.9	0
62	FLIPPED CLASSROOM AND GAMIFICATION IN THE TEACHING OF THE PHYSICS LABORATORY. EDULEARN Proceedings, 2022, , .	0.0	0