Laurent Pedesseau

List of Publications by Year
in descending order

95 papers	10,564 citations	159358 30 h-index	60497 81 g-index
98 all docs	98 docs citations	98 times ranked	10196 citing authors

#	Article	IF	Citations
1	Epitaxial IIIâ€“V/Si Vertical Heterostructures with Hybrid 2Dâ€Semimetal/Semiconductor Ambipolar and Photoactive Properties. Advanced Science, 2022, 9, e2101661.	5.6	13
2	Band gap, effective masses, and energy level alignment of 2D and 3D halide perovskites and heterostructures using DFT-1/2. Physical Review Materials, 2022, 6, .	0.9	13
3	Dangling Octahedra Enable Edge States in 2D Lead Halide Perovskites. Advanced Materials, 2022, 34, e2201666.	11.1	22
4	Pb-free halide perovskites for solar cells, light-emitting diodes, and photocatalysts. APL Materials, 2022, 10, .	2.2	11
5	Electronic structure and stability of Cs2TiX6 and Cs2ZrX6 (X = Br, I) vacancy ordered double perovskites. Applied Physics Letters, 2021, 119, .	1.5	28
6	Nonadiabatic molecular dynamics analysis of hybrid Dionâ€“Jacobson 2D leads iodide perovskites. Applied Physics Letters, 2021, 119, .	1.5	9
7	Importance of Vacancies and Doping in the Hole-Transporting Nickel Oxide Interface with Halide Perovskites. ACS Applied Materials & Interfaces, 2020, 12, 6633-6640.	4.0	21
8	Fully Inorganic Mixed Cation Lead Halide Perovskite Nanoparticles: A Study at the Atomic Level. Chemistry of Materials, 2020, 32, 1467-1474.	3.2	11
9	Strong Electronâ€“Phonon Interaction in 2D Vertical Homovalent IIIâ€“V Singularities. ACS Nano, 2020, 14, 13127-13136.	7.3	8
10	Charge carrier dynamics in two-dimensional hybrid perovskites: Dionâ€“Jacobson vs. Ruddlesdenâ€“Popper phases. Journal of Materials Chemistry A, 2020, 8, 22009-22022.	5.2	72
11	Negative Pressure Engineering with Large Cage Cations in 2D Halide Perovskites Causes Lattice Softening. Journal of the American Chemical Society, 2020, 142, 11486-11496.	6.6	84
12	Detrimental effects of ion migration in the perovskite and hole transport layers on the efficiency of inverted perovskite solar cells. Journal of Photonics for Energy, 2020, 10, 1.	0.8	3
13	Shape transition in InAs nanostructures formed by Stranski-Krastanow growth mode on InP (001) substrate. Applied Physics Letters, 2019, 114, .	1.5	8
14	Cation Alloying Delocalizes Polarons in Lead Halide Perovskites. Journal of Physical Chemistry Letters, 2019, 10, 3516-3524.	2.1	33
15	Structural and thermodynamic limits of layer thickness in 2D halide perovskites. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 58-66.	3.3	236
16	A study of the strain distribution by scanning X-ray diffraction on GaP/Si for IIIâ€“V monolithic integration on silicon. Journal of Applied Crystallography, 2019, 52, 809-815.	1.9	2
17	Hybrid Dionâ€“Jacobson 2D Lead Iodide Perovskites. Journal of the American Chemical Society, 2018, 140, 3775-3783.	6.6	686
18	Density of States Broadening in CH₃NH₃PbI₃ Hybrid Perovskites Understood from ab Initio Molecular Dynamics Simulations. ACS Energy Letters, 2018, 3, 787-793.	8.8	28

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19	Composite Nature of Layered Hybrid Perovskites: Assessment on Quantum and Dielectric Confinements and Band Alignment. ACS Nano, 2018, 12, 3321-3332.	7.3	146
20	Computational analysis of hybrid perovskite on silicon 2-T tandem solar cells based on a Si tunnel junction. Optical and Quantum Electronics, 2018, 50, 1.	1.5	26
21	A new approach to modelling Kelvin probe force microscopy of hetero-structures in the dark and under illumination. Optical and Quantum Electronics, 2018, 50, 1.	1.5	6
22	Anharmonicity and Disorder in the Black Phases of Cesium Lead Iodide Used for Stable Inorganic Perovskite Solar Cells. ACS Nano, 2018, 12, 3477-3486.	7.3	546
23	Transient simulation of halide perovskite-based solar cells with mobile ions and carriers. , 2018, , .		0
24	Anharmonicity and Disorder in the Black Phases of CsPbI3 used for Stable Inorganic Perovskite Solar Cells. , 2018, , .		1
25	Geometry Distortion and Small Polaron Binding Energy Changes with Ionic Substitution in Halide Perovskites. Journal of Physical Chemistry Letters, 2018, 9, 7130-7136.	2.1	52
26	Multiscale in modelling and validation for solar photovoltaics. EPJ Photovoltaics, 2018, 9, 10.	0.8	6
27	A Stressâ€Free and Textured GaP Template on Silicon for Solar Water Splitting. Advanced Functional Materials, 2018, 28, 1801585.	7.8	22
28	Concept of Lattice Mismatch and Emergence of Surface States in Two-dimensional Hybrid Perovskite Quantum Wells. Nano Letters, 2018, 18, 5603-5609.	4.5	103
29	Scaling law for excitons in 2D perovskite quantum wells. Nature Communications, 2018, 9, 2254.	5.8	559
30	Universal description of III-V/Si epitaxial growth processes. Physical Review Materials, 2018, 2, .	0.9	43
31	Extremely efficient internal exciton dissociation through edge states in layered 2D perovskites. Science, 2017, 355, 1288-1292.	6.0	830
32	Influence of Schottky contact on the C-V and J-V characteristics of HTM-free perovskite solar cells. EPJ Photovoltaics, 2017, 8, 85501.	0.8	19
33	Al₄SiC₄ vibrational properties: density functional theory calculations compared to Raman and infrared spectroscopy measurements. Journal of Raman Spectroscopy, 2017, 48, 891-896.	1.2	5
34	Computational design of high performance hybrid perovskite on silicon 2-T tandem solar cells based on a tunnel junction. , 2017, , .		2
35	Numerical simulation of HTM-free and WO<inf>x</inf> based perovskite cells: Effects of interface conditions. , 2017, , .		0
36	Decreasing the electronic confinement in layered perovskites through intercalation. Chemical Science, 2017, 8, 1960-1968.	3.7	114

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37	High-efficiency two-dimensional Ruddlesdenâ€“Popper perovskite solar cells. Nature, 2016, 536, 312-316.	13.7	2,767
38	Polaron Stabilization by Cooperative Lattice Distortion and Cation Rotations in Hybrid Perovskite Materials. Nano Letters, 2016, 16, 3809-3816.	4.5	245
39	Advances and Promises of Layered Halide Hybrid Perovskite Semiconductors. ACS Nano, 2016, 10, 9776-9786.	7.3	351
40	Quantum confinement and dielectric profiles of colloidal nanoplatelets of halide inorganic and hybrid organicâ€“inorganic perovskites. Nanoscale, 2016, 8, 6369-6378.	2.8	136
41	Theoretical insights into hybrid perovskites for photovoltaic applications. , 2016, , .		6
42	Dielectric properties of hybrid perovskites and drift-diffusion modeling of perovskite cells. Proceedings of SPIE, 2016, , .	0.8	8
43	Theoretical studies of Rashba and Dresselhaus effects in hybrid organic-inorganic perovskites for optoelectronic applications. , 2016, , .		2
44	Chapter 7. Electronic Properties of Metal Halide Perovskites. RSC Energy and Environment Series, 2016, , 202-233.	0.2	2
45	First-principles study of a sodium borosilicate glass-former. I. The liquid state. Physical Review B, 2015, 91, .	1.1	27
46	Al4SiC4 wurtzite crystal: Structural, optoelectronic, elastic, and piezoelectric properties. APL Materials, 2015, 3, .	2.2	14
47	Interplay of spinâ€“orbit coupling and lattice distortion in metal substituted 3D tri-chloride hybrid perovskites. Journal of Materials Chemistry A, 2015, 3, 9232-9240.	5.2	101
48	First-principles study of a sodium borosilicate glass-former. II. The glass state. Physical Review B, 2015, 91, .	1.1	33
49	Solid-State Physics Perspective on Hybrid Perovskite Semiconductors. Journal of Physical Chemistry C, 2015, 119, 10161-10177.	1.5	205
50	Ab initio calculations of polarization, piezoelectric constants, and elastic constants of InAs and InP in the wurtzite phase. Journal of Experimental and Theoretical Physics, 2015, 121, 246-249.	0.2	11
51	First-principles calculations of band offsets and polarization effects at InAs/InP interfaces. Journal Physics D: Applied Physics, 2015, 48, 355105.	1.3	4
52	Theoretical insights into multibandgap hybrid perovskites for photovoltaic applications. , 2015, , .		0
53	Rashba and Dresselhaus Effects in Hybrid Organicâ€“Inorganic Perovskites: From Basics to Devices. ACS Nano, 2015, 9, 11557-11567.	7.3	304
54	Density Functional Theory Simulations of Semiconductors for Photovoltaic Applications: Hybrid Organic-Inorganic Perovskites and III/V Heterostructures. International Journal of Photoenergy, 2014, 2014, 1-11.	1.4	23

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55	Electronic surface states and dielectric self-energy profiles in colloidal nanoscale platelets of CdSe. Physical Chemistry Chemical Physics, 2014, 16, 25182-25190.	1.3	30
56	Theoretical study of optical properties of anti phase domains in GaP. Journal of Applied Physics, 2014, 115, .	1.1	17
57	Monolithic Integration of Diluted-Nitride IIIâ€“V-N Compounds on Silicon Substrates: Toward the IIIâ€“V/Si Concentrated Photovoltaics. Energy Harvesting and Systems, 2014, 1, .	1.7	9
58	Theoretical insights into multibandgap hybrid perovskites for photovoltaic applications. Proceedings of SPIE, 2014, , .	0.8	9
59	Strain-induced fundamental optical transition in (In,Ga)As/GaP quantum dots. Applied Physics Letters, 2014, 104, 011908.	1.5	12
60	Analysis of Multivalley and Multibandgap Absorption and Enhancement of Free Carriers Related to Exciton Screening in Hybrid Perovskites. Journal of Physical Chemistry C, 2014, 118, 11566-11572.	1.5	463
61	Electronic properties of 2D and 3D hybrid organic/inorganic perovskites for optoelectronic and photovoltaic applications. Optical and Quantum Electronics, 2014, 46, 1225-1232.	1.5	60
62	DFT and k Â· p modelling of the phase transitions of lead and tin halide perovskites for photovoltaic cells. Physica Status Solidi - Rapid Research Letters, 2014, 8, 31-35.	1.2	177
63	Comment on â€œDensity functional theory analysis of structural and electronic properties of orthorhombic perovskite CH3NH3PbI3â€•by Y. Wang et al., Phys. Chem. Chem. Phys., 2014, 16, 1424â€“1429. Physical Chemistry Chemical Physics, 2014, 16, 8697-8698.	1.3	13
64	Composition dependent nature of the fundamental optical transition in (In, Ga)As/GaP quantum dots. , 2014, , .		0
65	Understanding Quantum Confinement of Charge Carriers in Layered 2D Hybrid Perovskites. ChemPhysChem, 2014, 15, 3733-3741.	1.0	211
66	Design of a lattice-matched IIIâ€“Vâ€“N/Si photovoltaic tandem cell monolithically integrated on silicon substrate. Optical and Quantum Electronics, 2014, 46, 1397-1403.	1.5	26
67	Importance of Spinâ€“Orbit Coupling in Hybrid Organic/Inorganic Perovskites for Photovoltaic Applications. Journal of Physical Chemistry Letters, 2013, 4, 2999-3005.	2.1	1,021
68	Vibrational properties of 2H-PbI2 semiconductors studied via Density Functional Theory calculations. Thin Solid Films, 2013, 541, 9-11.	0.8	6
69	Vibrational properties of SrCu2O2 studied via Density Functional Theory calculations and compared to Raman and infrared spectroscopy measurements. Thin Solid Films, 2013, 541, 113-116.	0.8	5
70	Raman investigation of GaPâ€“Si interfaces grown by molecular beam epitaxy. Thin Solid Films, 2013, 541, 72-75.	0.8	3
71	Evaluation of InGaPN and GaAsPN materials lattice-matched to Si for multi-junction solar cells. Journal of Applied Physics, 2013, 113, .	1.1	46
72	Optical, microstructural, vibrational, and theoretical studies of p-type SrCu2O2and BaCu2O2transparent conductive oxides. , 2013, , .		0

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73	Intrinsic optical confinement for ultrathin InAsN quantum well superlattices. , 2013, , .		0
74	First-principles density functional theory study of strained wurtzite InP and InAs. Journal Physics D: Applied Physics, 2013, 46, 505106.	1.3	14
75	Structural and optical properties of (In,Ga)As/GaP quantum dots and (GaAsPN/GaPN) diluted-nitride nanolayers coherently grown onto GaP and Si substrates for photonics and photovoltaics applications. , 2013, , .		0
76	Nonâ€linear electroâ€elastic coupling in highly strained zincâ€blende compounds: InGaP/GaP [111] quantum wells. Physica Status Solidi (B): Basic Research, 2013, 250, 765-768.	0.7	0
77	Non-linear electro-elastic coupling in non-centrosymmetric materials. Journal of Physics: Conference Series, 2012, 367, 012005.	0.3	1
78	Electronic model for self-assembled hybrid organic/perovskite semiconductors: Reverse band edge electronic states ordering and spin-orbit coupling. Physical Review B, 2012, 86, .	1.1	173
79	Theoretical and experimental studies of (In,Ga)As/GaP quantum dots. Nanoscale Research Letters, 2012, 7, 643.	3.1	4
80	On the entanglement of electrostriction and non-linear piezoelectricity in non-centrosymmetric materials. Applied Physics Letters, 2012, 100, .	1.5	29
81	30-band kâ‹…p method for quantum semiconductor heterostructures. Applied Physics Letters, 2011, 98, .	1.5	17
82	FeII/FeIII mixed-valence state induced by Li-insertion into the metal-organic-framework Mil53(Fe): A DFT+U study. Journal of Power Sources, 2011, 196, 3426-3432.	4.0	51
83	Design of Electrode Materials for Lithium-Ion Batteries: The Example of Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2010, 114, 9518-9527.	1.5	82
84	Analysis of carriers dynamics and laser emission in 1.55-Î¼m InAs/InP(113)B quantum dot lasers. Proceedings of SPIE, 2010, , .	0.8	1
85	Light emitting diodes on silicon substrates: preliminary results. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 2212-2216.	0.8	3
86	InAs QDs on InP: polarization insensitive SOA and non-radiative Auger processes. Optical and Quantum Electronics, 2008, 40, 1233-1238.	1.5	3
87	Mass and momentum interface equilibrium by molecular modeling. Simulating AFM adhesion between (120) gypsum faces in a saturated solution and consequences on gypsum cohesion. Cement and Concrete Research, 2008, 38, 290-299.	4.6	11
88	Semianalytical model for simulation of electronic properties of narrow-gap strained semiconductor quantum nanostructures. Physical Review B, 2008, 77, .	1.1	15
89	Polarization Insensibility of Columnar Quantum Dot Structure Emitting at : A Theoretical Study. Research Letters in Physics, 2008, 2008, 1-4.	0.2	0
90	Theoretical study of highly strained InAs material from first-principles modelling: application to an ideal QD. Journal Physics D: Applied Physics, 2008, 41, 165505.	1.3	13

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91	From kÂ·p to atomic calculations applied to semiconductor heterostructures. Journal of Physics: Conference Series, 2008, 107, 012009.	0.3	0
92	Semianalytical evaluation of linear and nonlinear piezoelectric potentials for quantum nanostructures with axial symmetry. Applied Physics Letters, 2007, 91, 122112.	1.5	21
93	Atomic Calculations Applied to Semiconductor Hetero Structures. AIP Conference Proceedings, 2007, , .	0.3	3
94	Phases, periphases, and interphases equilibrium by molecular modeling. I. Mass equilibrium by the semianalytical stochastic perturbations method and application to a solution between (120) gypsum faces. Journal of Chemical Physics, 2004, 121, 12511.	1.2	3
95	Partial stresses in heterogeneous media by a direct statistical approach. Comptes Rendus - Mecanique, 2004, 332, 305-312.	2.1	3