Samuel PoncÃ©

List of Publications by Year
in descending order

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44	9,158	159358	223531
papers	citations	30 h-index	46 g-index

46	46	46	10275
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Anisotropic-strain-enhanced hole mobility in GaN by lattice matching to ZnGeN2 and MgSiN2. Applied Physics Letters, 2022, 120, .	1.5	2
2	Limits to Electrical Mobility in Lead-Halide Perovskite Semiconductors. Journal of Physical Chemistry Letters, 2021, 12, 3607-3617.	2.1	45
3	Importance of Longâ€Range Channel Sr Displacements for the Narrow Emission in Sr[Li₂Al₂O₂N₂]:Eu²⁺Phosphor. Advanced Optical Materials, 2021, 9, 2100649.	3.6	10
4	Common workflows for computing material properties using different quantum engines. Npj Computational Materials, 2021, 7, .	3.5	10
5	Virtual Computational Chemistry Teaching Laboratoriesâ€”Hands-On at a Distance. Journal of Chemical Education, 2021, 98, 3163-3171.	1.1	15
6	Ultrafast photo-induced phonon hardening due to Pauli blocking in MAPbI₃ single-crystal and polycrystalline perovskites. JPhys Materials, 2021, 4, 044017.	1.8	4
7	First-principles predictions of Hall and drift mobilities in semiconductors. Physical Review Research, 2021, 3, .	1.3	48
8	Wannier90 as a community code: new features and applications. Journal of Physics Condensed Matter, 2020, 32, 165902.	0.7	807
9	First-principles calculations of charge carrier mobility and conductivity in bulk semiconductors and two-dimensional materials. Reports on Progress in Physics, 2020, 83, 036501.	8.1	176
10	Theory and Computation of Hall Scattering Factor in Graphene. Nano Letters, 2020, 20, 8861-8865.	4.5	13
11	Superconducting properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoTe</mml:mi><mml:mn>2</mml:mn></mml:msub><m from ab initio anisotropic Migdal-Eliashberg theory. Physical Review B, 2020, 101, .	1.1	10
12	Design rule for the emission linewidth of Eu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1136" altimg="si27.svg"><mml:msup><mml:mrow /><mml:mrow><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:math>-activated phosphors. Journal of Luminescence, 2020, 224, 117258.	1.5	7
13	Structural, electronic, elastic, power, and transport properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mtext>â€²</mml:mtext><mml:msub><mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>from first principles. Physical Review Research, 2020, 2, .	1.3	43
14	Beyond the one-dimensional configuration coordinate model of photoluminescence. Physical Review B, 2019, 100, .	1.1	10
15	Hole mobility of strained GaN from first principles. Physical Review B, 2019, 100, .	1.1	75
16	Route to High Hole Mobility in GaN via Reversal of Crystal-Field Splitting. Physical Review Letters, 2019, 123, 096602.	2.9	63
17	Ab initiotheory of polarons: Formalism and applications. Physical Review B, 2019, 99, .	1.1	84
18	Polarons from First Principles, without Supercells. Physical Review Letters, 2019, 122, 246403.	2.9	79

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19	Dimensional Crossover in the Carrier Mobility of Two-Dimensional Semiconductors: The Case of InSe. Nano Letters, 2019, 19, 1774-1781.	4.5	75
20	Origin of Low Carrier Mobilities in Halide Perovskites. ACS Energy Letters, 2019, 4, 456-463.	8.8	136
21	Electron-plasmon and electron-phonon satellites in the angle-resolved photoelectron spectra of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math> -doped anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2018, 97, .	1.1	27
22	Towards predictive many-body calculations of phonon-limited carrier mobilities in semiconductors. Physical Review B, 2018, 97, .	1.1	224
23	Carrier Lifetimes and Polaronic Mass Enhancement in the Hybrid Halide Perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi>CH</mml:mi></mml:mrow><mml:mrow><mml:mn>3 Physical Review Letters, 2018, 121, 086402.	2.9	76
24	Assessment of Firstâ€Principles and Semiempirical Methodologies for Absorption and Emission Energies of Ce³⁺â€Doped Luminescent Materials. Advanced Optical Materials, 2017, 5, 1600997.	3.6	35
25	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
26	Origin of Superconductivity and Latent Charge Density Wave in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>NbS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></m Physical Review Letters, 2017, 119, 087003.	2.9	108
27	First-principles study of the luminescence of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Eu</mml:mi></mml:mrow><mml:mrow><m -doped phosphors. Physical Review B, 2017, 96, .	1.1	44
28	Temperature Dependence of the Energy Levels of Methylammonium Lead Iodide Perovskite from First-Principles. Journal of Physical Chemistry Letters, 2016, 7, 5247-5252.	2.1	100
29	Recent developments in the ABINIT software package. Computer Physics Communications, 2016, 205, 106-131.	3.0	662
30	EPW: Electronâ€“phonon coupling, transport and superconducting properties using maximally localized Wannier functions. Computer Physics Communications, 2016, 209, 116-133.	3.0	777
31	First-principles study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mrow><mml:mi>Ce</mml:mi></mml:mrow><m silicate nitride phosphors: Neutral excitation, Stokes shift, and luminescent center identification. Physical Review B, 2016, 93, .	1.1	49
32	Precise effective masses from density functional perturbation theory. Physical Review B, 2016, 93, .	1.1	28
33	Understanding Thermal Quenching of Photoluminescence in Oxynitride Phosphors from First Principles. Journal of Physical Chemistry C, 2016, 120, 4040-4047.	1.5	58
34	Dynamical and anharmonic effects on the electron-phonon coupling and the zero-point renormalization of the electronic structure. Physical Review B, 2015, 92, .	1.1	104
35	Many-body perturbation theory approach to the electron-phonon interaction with density-functional theory as a starting point. Physical Review B, 2015, 91, .	1.1	46
36	Temperature dependence of the electronic structure of semiconductors and insulators. Journal of Chemical Physics, 2015, 143, 102813.	1.2	139

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37	Temperature dependence of electronic eigenenergies in the adiabatic harmonic approximation. Physical Review B, 2014, 90, .	1.1	91
38	First-principles characterization of the electronic and optical properties of hexagonal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si79.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">LiIO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mm Optical Materials, 2014, 36, 1494-1501.	1.7	13
39	Many-Body Effects on the Zero-Point Renormalization of the Band Structure. Physical Review Letters, 2014, 112, .	2.9	141
40	Verification of first-principles codes: Comparison of total energies, phonon frequencies, electronâ€“phonon coupling and zero-point motion correction to the gap between ABINIT and QE/Yambo. Computational Materials Science, 2014, 83, 341-348.	1.4	88
41	First-principles and experimental characterization of the electronic and optical properties of CaS and CaO. Optical Materials, 2013, 35, 1477-1480.	1.7	13
42	Quasiparticle electronic structure of barium-silicon oxynitrides for white-LED application. Physical Review B, 2013, 88, .	1.1	8
43	Band widths and gaps from the Tran-Blaha functional: Comparison with many-body perturbation theory. Physical Review B, 2013, 87, .	1.1	125
44	Interatomic potential to study plasticity in stainless steels: the FeNiCr model alloy. Modelling and Simulation in Materials Science and Engineering, 2011, 19, 085008.	0.8	183