Christopher E Patrick

List of Publications by Year
in descending order

32 papers	1,724 citations	394421 19 h-index	414414 32 g-index
32 all docs	32 docs citations	32 times ranked	2866 citing authors

#	Article	IF	Citations
1	MARMOT: magnetism, anisotropy, and more, using the relativistic disordered local moment picture at finite temperature. Electronic Structure, 2022, 4, 017001.	2.8	5
2	Ab initio calculations of the phase behavior and subsequent magnetostriction of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Fe</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">Ga</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math> within the disordered local moment picture. Physical Review B, 2021, 103, .	3.2	7
3	Extracting band-tail interface state densities from measurements and modelling of space charge layer resistance. Solar Energy Materials and Solar Cells, 2021, 231, 111307.	6.2	7
4	Spin Orientation and Magnetostriction of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi>Tb</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:m from First Principles. Physical Review Applied, 2020, 14, .	3.8	11
5	Temperature-dependent spin polarization of Heusler <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Co</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>MnSi</mml:mi></mml:math> from the disordered local-moment approach: Effects of atomic disordering and nonstoichiometry. Physical Review B, 2020, 102, .	3.2	14
6	Tunability of the spin reorientation transitions with pressure in NdCo5. Applied Physics Letters, 2020, 116, 102408.	3.3	2
7	Torque magnetometry study of the spin reorientation transition and temperature-dependent magnetocrystalline anisotropy in NdCo₅. Journal of Physics Condensed Matter, 2020, 32, 255802.	1.8	8
8	First-principles calculations of the magnetocrystalline anisotropy of the prototype 2:17 cell boundary phaseYCo1-x-yFexCuy5. Journal of Magnetism and Magnetic Materials, 2019, 477, 147-155.	2.3	9
9	Ab initio calculations of temperature-dependent magnetostriction of Fe and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>A</mml:mi><mml:mn>2</mml:mn></mml:mrow><mml:m width="4pt" /><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:m within the disordered local moment picture. Physical Review B, 2019, 99, .	3.2	15
10	Crystal field coefficients for yttrium analogues of rare-earth/transition-metal magnets using density-functional theory in the projector-augmented wave formalism. Journal of Physics Condensed Matter, 2019, 31, 305901.	1.8	9
11	Beyond the RPA and GW methods with adiabatic xc-kernels for accurate ground state and quasiparticle energies. Npj Computational Materials, 2019, 5, .	8.7	33
12	Structural and magnetic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>GdCo</mml:mi><mml:mrow><mml:mn>5</mml:mn></ Physical Review Materials, 2019, 3, .	2.4	8
13	Temperature-dependent magnetocrystalline anisotropy of rare earth/transition metal permanent magnets from first principles: The light <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>R</mml:mi><mml:msub><mml:mi>Co</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:mrow></mml:math> intermetallics. Physical Review Materials, 2019, 3, .	2.4	27
14	Calculating the Magnetic Anisotropy of Rare-Earthâ€“Transition-Metal Ferrimagnets. Physical Review Letters, 2018, 120, 097202.	7.8	34
15	Field-induced canting of magnetic moments in GdCo5 at finite temperature: first-principles calculations and high-field measurements. Journal of Physics Condensed Matter, 2018, 30, 32LT01.	1.8	4
16	Rare-earth/transition-metal magnets at finite temperature: Self-interaction-corrected relativistic density functional theory in the disordered local moment picture. Physical Review B, 2018, 97, .	3.2	31
17	Simple vertex correction improves <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m band energies of bulk and two-dimensional crystals. Physical Review B, 2017, 96, .	3.2	37
18	Rare-earth/transition-metal magnetic interactions in pristine and (Ni,Fe)-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>YCo</mml:mi><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>GdCo</mml:mi><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub></mml:math>. Physical Review Materials, 2017, 1, .	2.4	31

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19	xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mtext>Hubbard-</mml:mtext><mml:mi>U</mml:mi></mml:m Hamiltonians for non-self-consistent random-phase approximation total-energy calculations: A study of ZnS,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>TiO</mml:mtext><mml:mn>2</mml:mn></mml:msub and NiO. Physical Review B, 2016, 93, .	3.2	19
20	Stochastic Approach to Phonon-Assisted Optical Absorption. Physical Review Letters, 2015, 115, 177401.	7.8	85
21	Anharmonic stabilization and band gap renormalization in the perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CsSnI</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:m Physical Review B, 2015, 92, .	3.2	76
22	Adiabatic-connection fluctuation-dissipation DFT for the structural properties of solidsâ€"The renormalized ALDA and electron gas kernels. Journal of Chemical Physics, 2015, 143, 102802.	3.0	56
23	Unified theory of electronâ€“phonon renormalization and phonon-assisted optical absorption. Journal of Physics Condensed Matter, 2014, 26, 365503.	1.8	47
24	Atomic-Scale Observation of Multiconformational Binding and Energy Level Alignment of Ruthenium-Based Photosensitizers on TiO₂ Anatase. Nano Letters, 2014, 14, 563-569.	9.1	67
25	Structure of a Water Monolayer on the Anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn><mml:m stretchy="false">(</mml:mo><mml:mn>101</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 487 Td (stretchy="fals	3.8	42
26	TiO₂ Anatase with a Bandgap in the Visible Region. Nano Letters, 2014, 14, 6533-6538.	9.1	531
27	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>quasiparticle band structures of stibnite, antimonselite, bismuthinite, and guanajuatite. Physical Review B, 2013, 87, .	3.2	178
28	Quantum nuclear dynamics in the photophysics of diamondoids. Nature Communications, 2013, 4, 2006.	12.8	88
29	Quantitative Analysis of Valence Photoemission Spectra and Quasiparticle Excitations at Chromophore-Semiconductor Interfaces. Physical Review Letters, 2012, 109, 116801.	7.8	26
30	GW quasiparticle bandgaps of anatase TiO₂starting from DFT +U. Journal of Physics Condensed Matter, 2012, 24, 202201.	1.8	67
31	Structural and Electronic Properties of Semiconductorâ€Sensitized Solarâ€Cell Interfaces. Advanced Functional Materials, 2011, 21, 4663-4667.	14.9	131
32	O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:mi>s</mml:mi></mml:mrow></mml:math>core-level shifts at the anatase TiO<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>(101)/N3 photovoltaic interface: Signature of H-bonded supramolecular assembly. Physical Review B, 2011, 84, .	3.2	24