John C Thomas

List of Publications by Year
in descending order

29	1,249	471509 17	501196 28
papers	citations	h-index	g-index

31	31	31	1713
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Comparing crystal structures with symmetry and geometry. Npj Computational Materials, 2021, 7, .	8.7	21
2	Order-disorder versus displacive transitions in Jahn-Teller active layered materials. Physical Review Materials, 2020, 4, .	2.4	17
3	Discovering hierarchies among intermetallic crystal structures. Physical Review Materials, 2020, 4, .	2.4	9
4	Machine learning the density functional theory potential energy surface for the inorganic halide perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">CsPbBr</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2019, 100, .	3.2	14
5	Finite-temperature simulation of anharmonicity and octahedral tilting transitions in halide perovskites. Physical Review Materials, 2019, 3, .	2.4	28
6	First-Principles Statistical Mechanics of Multicomponent Crystals. Annual Review of Materials Research, 2018, 48, 27-55.	9.3	98
7	Hamiltonians and order parameters for crystals of orientable molecules. Physical Review B, 2018, 98, .	3.2	9
8	PRISMS: An Integrated, Open-Source Framework for Accelerating Predictive Structural Materials Science. Jom, 2018, 70, 2298-2314.	1.9	30
9	Order parameters for symmetry-breaking structural transitions: The tetragonal-monoclinic transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZrO</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2017, 96, .	3.2	12
10	Symmetry-adapted order parameters and free energies for solids undergoing order-disorder phase transitions. Physical Review B, 2017, 96, .	3.2	33
11	The exploration of nonlinear elasticity and its efficient parameterization for crystalline materials. Journal of the Mechanics and Physics of Solids, 2017, 107, 76-95.	4.8	36
12	Integrated Computational Modeling of Water Side Corrosion in Zirconium Metal Clad Under Nominal LWR Operating Conditions. Jom, 2016, 68, 2900-2911.	1.9	13
13	Effects of strain on the stability of tetragonal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>ZrO</mml:mtext><mml:mn>2</mml:mn></mml:ms Physical Review B, 2016, 94, .	3.2	18
14	First-principles survey of the structure, formation energies, and transition levels of As-interstitial defects in InGaAs. Physical Review B, 2015, 92, .	3.2	7
15	Phase stability analysis of the InAs/GaAs (001) wetting layer from first principles. Physical Review B, 2014, 89, .	3.2	1
16	Elastic properties and stress-temperature phase diagrams of high-temperature phases with low-temperature lattice instabilities. Physical Review B, 2014, 90, .	3.2	23
17	Low-temperature structural and transport anomalies in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Se</mml:mi></mml:math>. Physical Review B, 2014, 89, .	3.2	54
18	Designing the next generation high capacity battery electrodes. Energy and Environmental Science, 2014, 7, 1760.	30.8	104

#	Article	IF	Citations
19	Finite-temperature properties of strongly anharmonic and mechanically unstable crystal phases from first principles. Physical Review B, 2013, 88, .	3.2	138
20	Bismuth-containing IIIâ€“V semiconductors. , 2013, , 139-158.		6
21	Considerations for surface reconstruction stability prediction on GaAs(001). Physical Review B, 2013, 87, .	3.2	8
22	Surface reconstruction stability and configurational disorder on Bi-terminated GaAs(001). Physical Review B, 2013, 87, .	3.2	22
23	Surface structure of bismuth terminated GaAs surfaces grown with molecular beam epitaxy. Surface Science, 2012, 606, 1203-1207.	1.9	27
24	Configuring pnicogen rings in skutterudites for low phonon conductivity. Physical Review B, 2012, 86, .	3.2	30
25	Linking the electronic structure of solids to their thermodynamic and kinetic properties. Mathematics and Computers in Simulation, 2010, 80, 1393-1410.	4.4	160
26	Structural Order-Disorder Transitions and Phonon Conductivity of Partially Filled Skutterudites. Physical Review Letters, 2010, 105, 265901.	7.8	56
27	Systematic approach for determination of equilibrium atomic surface structure. Physical Review B, 2010, 82, .	3.2	24
28	Surface atomic order of compound III-V semiconductor alloys at finite temperature. Physical Review B, 2009, 80, .	3.2	10
29	Nondilute diffusion from first principles: Li diffusion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Li</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub> Physical Review B, 2008, 78, .	3.2	224