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	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
2	Linking the electronic structure of solids to their thermodynamic and kinetic properties. Mathematics and Computers in Simulation, 2010, 80, 1393-1410.	4.4	160
3	Finite-temperature properties of strongly anharmonic and mechanically unstable crystal phases from first principles. Physical Review B, 2013, 88, .	3.2	138
4	Designing the next generation high capacity battery electrodes. Energy and Environmental Science, 2014, 7, 1760.	30.8	104
5	First-Principles Statistical Mechanics of Multicomponent Crystals. Annual Review of Materials Research, 2018, 48, 27-55.	9.3	98
6	Structural Order-Disorder Transitions and Phonon Conductivity of Partially Filled Skutterudites. Physical Review Letters, 2010, 105, 265901.	7.8	56
7	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
8	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
9	Symmetry-adapted order parameters and free energies for solids undergoing order-disorder phase transitions. Physical Review B, 2017, 96, .	3.2	33
10	Configuring pnicogen rings in skutterudites for low phonon conductivity. Physical Review B, 2012, 86, .	3.2	30
11	PRISMS: An Integrated, Open-Source Framework for Accelerating Predictive Structural Materials Science. Jom, 2018, 70, 2298-2314.	1.9	30
12	Finite-temperature simulation of anharmonicity and octahedral tilting transitions in halide perovskites. Physical Review Materials, 2019, 3, .	2.4	28
13	Surface structure of bismuth terminated GaAs surfaces grown with molecular beam epitaxy. Surface Science, 2012, 606, 1203-1207.	1.9	27
14	Systematic approach for determination of equilibrium atomic surface structure. Physical Review B, 2010, 82, .	3.2	24
15	Elastic properties and stress-temperature phase diagrams of high-temperature phases with low-temperature lattice instabilities. Physical Review B, 2014, 90, .	3.2	23
16	Surface reconstruction stability and configurational disorder on Bi-terminated GaAs(001). Physical Review B, 2013, 87, .	3.2	22
17	Comparing crystal structures with symmetry and geometry. Npj Computational Materials, 2021, 7, .	8.7	21
18	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:msub> Physical Review B, 2016, 94, .	3.2	18

#	Article	IF	Citations
19	Order-disorder versus displacive transitions in Jahn-Teller active layered materials. Physical Review Materials, 2020, 4, .	2.4	17
20	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
21	Integrated Computational Modeling of Water Side Corrosion in Zirconium Metal Clad Under Nominal LWR Operating Conditions. Jom, 2016, 68, 2900-2911.	1.9	13
22	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></mm Physical Review B, 2017, 96, .	3.2	12
23	Surface atomic order of compound III-V semiconductor alloys at finite temperature. Physical Review B, 2009, 80, .	3.2	10
24	Hamiltonians and order parameters for crystals of orientable molecules. Physical Review B, 2018, 98, .	3.2	9
25	Discovering hierarchies among intermetallic crystal structures. Physical Review Materials, 2020, 4, .	2.4	9
26	Considerations for surface reconstruction stability prediction on GaAs(001). Physical Review B, 2013, 87, .	3.2	8
27	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
28	Bismuth-containing IIIâ€“V semiconductors. , 2013, , 139-158.		6
29	Phase stability analysis of the InAs/GaAs (001) wetting layer from first principles. Physical Review B, 2014, 89, .	3.2	1