James E Saal

List of Publications by Year
in descending order

57	5,635	147726	149623
papers	citations	31 h-index	56 g-index

59	59	59	5501
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Materials Design and Discovery with High-Throughput Density Functional Theory: The Open Quantum Materials Database (OQMD). Jom, 2013, 65, 1501-1509.	0.9	1,461
2	The Open Quantum Materials Database (OQMD): assessing the accuracy of DFT formation energies. Npj Computational Materials, 2015, 1, .	3.5	1,200
3	Combinatorial screening for new materials in unconstrained composition space with machine learning. Physical Review B, 2014, 89, .	1.1	527
4	High-Throughput Computational Screening of Perovskites for Thermochemical Water Splitting Applications. Chemistry of Materials, 2016, 28, 5621-5634.	3.2	191
5	Enthalpies of formation of magnesium compounds from first-principles calculations. Intermetallics, 2009, 17, 878-885.	1.8	159
6	Passivation of a corrosion resistant high entropy alloy in non-oxidizing sulfate solutions. Acta Materialia, 2019, 164, 362-376.	3.8	145
7	Thermodynamic stability of Mg-based ternary long-period stacking ordered structures. Acta Materialia, 2014, 68, 325-338.	3.8	134
8	Predicting Î²â€² precipitate morphology and evolution in Mgâ€“RE alloys using a combination of first-principles calculations and phase-field modeling. Acta Materialia, 2014, 76, 259-271.	3.8	93
9	Computational materials design of a corrosion resistant high entropy alloy for harsh environments. Scripta Materialia, 2018, 153, 19-22.	2.6	93
10	Formation of high-strength <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si4.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mi>Î²</mml:mi></mml:mrow><mml:mrow><mml:mo>â€²</mml:mo></ precipitates in Mgâ€“RE alloys: The role of the Mg/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif" overflow="scroll"><mml:mrow><mml:msup><mml:mrow><mml:mi>Î²</mml:mi></mml:mrow><mml:mrow><mml:mo>â€³</mml:mo></	3.8	88
11	High-throughput computational search for strengthening precipitates in alloys. Acta Materialia, 2016, 102, 125-135.	3.8	83
12	Equilibrium high entropy alloy phase stability from experiments and thermodynamic modeling. Scripta Materialia, 2018, 146, 5-8.	2.6	83
13	Thermodynamic stability of Coâ€“Alâ€“W L12 Î³â€². Acta Materialia, 2013, 61, 2330-2338.	3.8	76
14	Approaching chemical accuracy with density functional calculations: Diatomic energy corrections. Physical Review B, 2013, 87, .	1.1	75
15	Localized corrosion behavior of a single-phase non-equimolar high entropy alloy. Electrochimica Acta, 2019, 306, 71-84.	2.6	75
16	Machine Learning in Materials Discovery: Confirmed Predictions and Their Underlying Approaches. Annual Review of Materials Research, 2020, 50, 49-69.	4.3	75
17	Physical factors controlling the observed high-strength precipitate morphology in Mgâ€“rare earth alloys. Acta Materialia, 2014, 65, 240-250.	3.8	69
18	Prediction of seebeck coefficient for compounds without restriction to fixed stoichiometry: A machine learning approach. Journal of Computational Chemistry, 2018, 39, 191-202.	1.5	65

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19	Aqueous passivation of multi-principal element alloy Ni38Fe20Cr22Mn10Co10: Unexpected high Cr enrichment within the passive film. Acta Materialia, 2020, 198, 121-133.	3.8	64
20	The structural evolution of boron carbide via ab initio calculations. Applied Physics Letters, 2007, 91, .	1.5	61
21	Controlling the corrosion resistance of multi-principal element alloys. Scripta Materialia, 2020, 188, 96-101.	2.6	58
22	First-principles lattice dynamics and heat capacity of BiFeO3. Acta Materialia, 2011, 59, 4229-4234.	3.8	55
23	Thermodynamic stability of Mgâ€“Yâ€“Zn long-period stacking ordered structures. Scripta Materialia, 2012, 67, 798-801.	2.6	53
24	Soluteâ€“vacancy binding of the rare earths in magnesium from first principles. Acta Materialia, 2012, 60, 5151-5159.	3.8	50
25	Electrochemical metrics for corrosion resistant alloys. Scientific Data, 2021, 8, 58.	2.4	46
26	Computational design and initial corrosion assessment of a series of non-equimolar high entropy alloys. Scripta Materialia, 2019, 172, 12-16.	2.6	44
27	Energetics of antiphase boundaries in Î³â€² Co3(Al,W)-based superalloys. Acta Materialia, 2016, 103, 57-62.	3.8	40
28	Thermodynamic modeling of the Cuâ€“Si system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 520-526.	0.7	35
29	Crystal structure, energetics, and phase stability of strengthening precipitates in Mg alloys: A first-principles study. Acta Materialia, 2018, 158, 65-78.	3.8	35
30	Broken symmetry, strong correlation, and splitting between longitudinal and transverse optical phonons of MnO and NiO from first principles. Physical Review B, 2010, 82, .	1.1	31
31	Magnetic thermodynamics of fcc Ni from first-principles partition function approach. Journal of Applied Physics, 2010, 108, .	1.1	31
32	Strategies for accelerating the adoption of materials informatics. MRS Bulletin, 2018, 43, 683-689.	1.7	29
33	Thermodynamic modeling of fcc order/disorder transformations in the Coâ€“Pt system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 323-330.	0.7	25
34	Machine-Learning Guided Quantum Chemical and Molecular Dynamics Calculations to Design Novel Hole-Conducting Organic Materials. Journal of Physical Chemistry A, 2020, 124, 8330-8340.	1.1	25
35	Magnetic perturbation and associated energies of the antiphase boundaries in ordered Ni3Al. Journal of Applied Physics, 2010, 108, .	1.1	23
36	ICME Design of a Castable, Creep-Resistant, Single-Crystal Turbine Alloy. Jom, 2017, 69, 880-885.	0.9	19

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37	Effects of carbon in MgB2 thin films: Intrinsic or extrinsic. Applied Physics Letters, 2007, 90, 151920.	1.5	18
38	Communicationâ€"Dissolution and Passivation of a Ni-Cr-Fe-Ru-Mo-W High Entropy Alloy by Elementally Resolved Electrochemistry. Journal of the Electrochemical Society, 2020, 167, 061505.	1.3	18
39	Thermodynamic Properties of Co₃O₄and Sr₆Co₅O₁₅from First-Principles. Inorganic Chemistry, 2010, 49, 10291-10298.	1.9	17
40	Element redistributions during early stages of oxidation in a Ni38Cr22Fe20Mn10Co10 multi-principal element alloy. Scripta Materialia, 2021, 194, 113609.	2.6	16
41	Potential Dependent Mn Oxidation and Its Role in Passivation of Ni₃₈Fe₂₀Cr₂₂Mn₁₀Co₁₀Multi-Principal Element Alloy Using Multi-Element Resolved Atomic Emission Spectroelectrochemistry. Journal of the Electrochemical Society, 2021, 168, 051508.	1.3	15
42	Defects in boron carbide: First-principles calculations and CALPHAD modeling. Acta Materialia, 2012, 60, 7207-7215.	3.8	14
43	Phonon dispersion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Sr</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> by a first-principles cumulative force-constant approach. Physical Review B, 2010, 82, .	1.1	13
44	First-Principles Calculations and Thermodynamic Modeling of the Al2O3-Nd2O3System. Journal of the American Ceramic Society, 2008, 91, 3355-3361.	1.9	12
45	Firstâ€Principles Thermochemistry and Thermodynamic Modeling of the Al₂O₃â€"Nd₂O₃â€"SiO₂â€"Y₂O₃ Pseudoquaternary System. Journal of the American Ceramic Society, 2010, 93, 4158-4167.	1.9	12
46	Magnetic phase transformations of face-centered cubic and hexagonal close-packed Co at zero Kelvin. Journal of Physics Condensed Matter, 2010, 22, 096006.	0.7	12
47	Thermodynamic modeling of the PbX (X=S,Te) phase diagram using a five sub-lattice and two sub-lattice model. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 58, 17-24.	0.7	11
48	A first-principles scheme to phonons of high temperature phase: No imaginary modes for cubic SrTiO3. Applied Physics Letters, 2010, 97, 162907.	1.5	10
49	First-principles calculations and thermodynamic modeling of the Reâ€"Y system with extension to the Niâ€"Reâ€"Y system. Intermetallics, 2010, 18, 2412-2418.	1.8	10
50	Reflections on one million compounds in the open quantum materials database (OQMD). JPhys Materials, 2022, 5, 031001.	1.8	9
51	THE IMPACT OF ACCEPTOR DOPANT MAGNESIUM AND OXYGEN VACANCY DEFECTS ON THE LATTICE OF BARIUM STRONTIUM TITANATE. Integrated Ferroelectrics, 2008, 101, 142-151.	0.3	8
52	Using First-Principles Calculations in CALPHAD Models to Determine Carrier Concentration of the Binary PbSe Semiconductor. Journal of Electronic Materials, 2019, 48, 1031-1043.	1.0	8
53	Effects of spin structures on Fermi surface topologies in BaFe2As2. Solid State Communications, 2011, 151, 272-275.	0.9	7
54	Summary of the CALPHAD XXXVI 2007 conference. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 9-31.	0.7	3

#	Article	IF	Citations
55	Overview: Age-Hardenable Microalloying in Magnesium. Jom, 2015, 67, 2425-2426.	0.9	3
56	Materials informatics and sustainabilityâ€"The case for urgency. Data-Centric Engineering, 2021, 2, .	1.2	2
57	Dynamic Properties of Magnesium Alloys. Jom, 2014, 66, 275-276.	0.9	0