Michael J Mehl

List of Publications by Year
in descending order

65 papers	8,224 citations	147801 31 h-index	133252 59 g-index
65 all docs	65 docs citations	65 times ranked	7701 citing authors

#	Article	IF	Citations
1	AFLOW-XtalFinder: a reliable choice to identify crystalline prototypes. Npj Computational Materials, 2021, 7, .	8.7	28
2	Automated coordination corrected enthalpies with AFLOW-CCE. Physical Review Materials, 2021, 5, .	2.4	9
3	Tin-pest problem as a test of density functionals using high-throughput calculations. Physical Review Materials, 2021, 5, .	2.4	7
4	Settling the matter of the role of vibrations in the stability of high-entropy carbides. Nature Communications, 2021, 12, 5747.	12.8	28
5	The AFLOW Library of Crystallographic Prototypes: Part 3. Computational Materials Science, 2021, 199, 110450.	3.0	16
6	The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812.		4
7	The AFLOW Library of Crystallographic Prototypes: Part 2. Computational Materials Science, 2019, 161, S1-S1011.	3.0	70
8	Theoretical studies of the vibrational properties of octahedrane (C12H12): A polyhedral caged hydrocarbon molecule. Journal of Chemical Physics, 2019, 150, 214304.	3.0	0
9	The AFLOW Fleet for Materials Discovery. , 2019, , 1-28.		0
10	A Brief History of Strukturbericht Symbols and Other Crystallographic Classification Schemes. Journal of Physics: Conference Series, 2019, 1290, 012016.	0.4	7
11	Bright triplet excitons in caesium lead halide perovskites. Nature, 2018, 553, 189-193.	27.8	716
12	AFLOW-SYM: platform for the complete, automatic and self-consistent symmetry analysis of crystals. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, 184-203.	0.1	44
13	The AFLOW Fleet for Materials Discovery. , 2018, , 1-28.		9
14	AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis. Journal of Chemical Information and Modeling, 2018, 58, 2477-2490.	5.4	69
15	Active bialkali photocathodes on free-standing graphene substrates. Npj 2D Materials and Applications, 2017, 1, .	7.9	24
16	The AFLOW Library of Crystallographic Prototypes: Part 1. Computational Materials Science, 2017, 136, S1-S828.	3.0	147
17	The AFLOW standard for high-throughput materials science calculations. Computational Materials Science, 2015, 108, 233-238.	3.0	244
18	Finding the stable structures of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mtext>N</mml:mtext><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> anab initiohigh-throughput approach. Physical Review B, 2015, 91, .	3.2	54

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19	Tight-Binding study of Boron structures. Journal of Physics and Chemistry of Solids, 2014, 75, 1106-1112.	4.0	4
20	Epitaxial Growth of Cubic and Hexagonal InN Thin Films via Plasma-Assisted Atomic Layer Epitaxy. Crystal Growth and Design, 2013, 13, 1485-1490.	3.0	45
21	AFLOW: An automatic framework for high-throughput materials discovery. Computational Materials Science, 2012, 58, 218-226.	3.0	898
22	Density functional study of the L10â€“Î±IrV transition in IrV and RhV. Journal of Alloys and Compounds, 2011, 509, 560-567.	5.5	1
23	Nearly metastable rhombohedral phases of bcc metals. Physical Review B, 2008, 77, .	3.2	4
24	Electronic structure and superconducting properties of lanthanum. Physical Review B, 2008, 78, .	3.2	20
25	Calculations of superconducting properties in yttrium and calcium under high pressure. Physical Review B, 2007, 75, .	3.2	32
26	A Tight-Binding Hamiltonian for Band Structure and Carrier Transport in Graphene Nanoribbons. Materials Research Society Symposia Proceedings, 2007, 1057, 1.	0.1	1
27	Calculations of the superconducting properties of scandium under high pressure. Physical Review B, 2007, 76, .	3.2	15
28	Phase stability in the Feâ€“Ni system: Investigation by first-principles calculations and atomistic simulations. Acta Materialia, 2005, 53, 4029-4041.	7.9	262
29	Theoretical confirmation of the experimental Raman spectra of the lower-order diamondoid molecule: cyclohexamantane (C26H30). Chemical Physics Letters, 2005, 403, 83-88.	2.6	21
30	Tetragonal Phase Transformation in Gold Nanowires. Journal of Engineering Materials and Technology, Transactions of the ASME, 2005, 127, 417-422.	1.4	44
31	Tight-Binding Total Energy Methods for Magnetic Materials and Multi-Element Systems. , 2005, , 275-305.		1
32	Consequences of zero-point motion to the radial distribution function of amorphous silicon. Journal of Physics Condensed Matter, 2004, 16, S5165-S5172.	1.8	7
33	Absence of metastable states in strained monatomic cubic crystals. Physical Review B, 2004, 70, .	3.2	29
34	Interlayer surface relaxations and energies of fcc metal surfaces by a tight-binding method. Physical Review B, 2004, 70, .	3.2	29
35	Stability and Structural Transition of Gold Nanowires under Their Own Surface Stresses. Materials Research Society Symposia Proceedings, 2004, 854, U5.7.1.	0.1	0
36	Application of a tight-binding total-energy method for FeAl. Journal of Physics Condensed Matter, 2002, 14, 1895-1902.	1.8	13

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37	Electronic structure calculations of lead chalcogenides PbS, PbSe, PbTe. Journal of Physics and Chemistry of Solids, 2002, 63, 833-841.	4.0	143
38	Tight-binding Hamiltonians for realistic electronic structure calculations. Physica B: Condensed Matter, 2001, 296, 129-137.	2.7	9
39	Occupation-number broadening schemes: Choice of â€œtemperatureâ€• Physical Review B, 2000, 61, 1654-1657.	3.2	19
40	Tight-binding study of stacking fault energies and the Rice criterion of ductility in the fcc metals. Physical Review B, 2000, 61, 4894-4897.	3.2	85
41	Ab InitioBased Tight-Binding Hamiltonian for the Dissociation of Molecules at Surfaces. Physical Review Letters, 1999, 82, 1209-1212.	7.8	36
42	Interatomic potentials for monoatomic metals from experimental data andab initiocalculations. Physical Review B, 1999, 59, 3393-3407.	3.2	1,231
43	Application of a tight-binding total-energy method for Al, Ga, and In. Physical Review B, 1998, 57, R2013-R2016.	3.2	40
44	Applications of a tight-binding total-energy method for transition and noble metals: Elastic constants, vacancies, and surfaces of monatomic metals. Physical Review B, 1996, 54, 4519-4530.	3.2	550
45	Development of a Kohn-Sham like potential in the self-consistent atomic deformation model. Journal of Physics and Chemistry of Solids, 1996, 57, 1405-1407.	4.0	17
46	A Model to Compute Phase Diagrams in Oxides with Empirical or First-Principles Energy Methods and Application to the Solubility Limits in the CaO-MgO System. Journal of the American Ceramic Society, 1996, 79, 2033-2040.	3.8	66
47	Spherical self-consistent atomic deformation model for first-principles energy calculations in ionic crystalline solids. Physical Review B, 1996, 54, 7729-7736.	3.2	19
48	First-Principles Calculation of the Structure of Mercury. Materials Research Society Symposia Proceedings, 1995, 408, 383.	0.1	1
49	Tight-binding total-energy method for transition and noble metals. Physical Review B, 1994, 50, 14694-14697.	3.2	258
50	Understanding The Nb-Ti-A1 System: First Principles Calculations. Materials Research Society Symposia Proceedings, 1994, 364, 1265.	0.1	1
51	Pressure dependence of the elastic moduli in aluminum-rich Al-Li compounds. Physical Review B, 1993, 47, 2493-2500.	3.2	397
52	Phase stability of wÃ¼stite at high pressure from first-principles linearized augmented plane-wave calculations. Physical Review B, 1993, 47, 7720-7731.	3.2	56
53	All-electron first-principles supercell total-energy calculation of the vacancy formation energy in aluminium. Physica B: Condensed Matter, 1991, 172, 211-215.	2.7	44
54	Calculation of energy barriers for physically allowed lattice-invariant strains in aluminum and iridium. Physical Review B, 1991, 43, 9498-9502.	3.2	28

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55	First-principles calculation of the elastic moduli ofNi3Al. Physical Review B, 1991, 43, 1805-1807.	3.2	31
56	New low-energy crystal structure for silicon. Physical Review Letters, 1991, 67, 715-718.	7.8	97
57	First Principles Calculations of the Equilibrium Mechanical Properties of Simple Metals and Ordered Intermetallic Alloys. Materials Research Society Symposia Proceedings, 1990, 186, 277.	0.1	12
58	Calculated elastic and thermal properties of MGO at high pressures and temperatures. Journal of Geophysical Research, 1990, 95, 7055-7067.	3.3	154
59	Structural properties of ordered high-melting-temperature intermetallic alloys from first-principles total-energy calculations. Physical Review B, 1990, 41, 10311-10323.	3.2	386
60	Potential-induced breathing model for the elastic moduli and high-pressure behavior of the cubic alkaline-earth oxides. Physical Review B, 1986, 33, 8685-8696.	3.2	185
61	Beyond the Rigid-Ion Approximation with Spherically Symmetric Ions. Physical Review Letters, 1985, 54, 1940-1943.	7.8	85
62	Beyond the local-density approximation in calculations of ground-state electronic properties. Physical Review B, 1983, 28, 1809-1834.	3.2	1,019
63	Easily Implementable Nonlocal Exchange-Correlation Energy Functional. Physical Review Letters, 1981, 47, 446-450.	7.8	298
64	Quantum theory of neutral-atom scattering at long range from solid cylinders. Physical Review A, 1980, 21, 1177-1184.	2.5	12
65	The Van der Waals interaction between an atom and a solid. Surface Science, 1980, 99, 553-569.	1.9	43