Michael J Mehl

List of Publications by Year
in descending order

65 papers	8,224 citations	147566 31 h-index	133063 59 g-index
65 all docs	65 docs citations	65 times ranked	7701 citing authors

#	Article	IF	Citations
1	Interatomic potentials for monoatomic metals from experimental data andab initiocalculations. Physical Review B, 1999, 59, 3393-3407.	1.1	1,231
2	Beyond the local-density approximation in calculations of ground-state electronic properties. Physical Review B, 1983, 28, 1809-1834.	1.1	1,019
3	AFLOW: An automatic framework for high-throughput materials discovery. Computational Materials Science, 2012, 58, 218-226.	1.4	898
4	Bright triplet excitons in caesium lead halide perovskites. Nature, 2018, 553, 189-193.	13.7	716
5	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.	1.1	550
6	Pressure dependence of the elastic moduli in aluminum-rich Al-Li compounds. Physical Review B, 1993, 47, 2493-2500.	1.1	397
7	Structural properties of ordered high-melting-temperature intermetallic alloys from first-principles total-energy calculations. Physical Review B, 1990, 41, 10311-10323.	1.1	386
8	Easily Implementable Nonlocal Exchange-Correlation Energy Functional. Physical Review Letters, 1981, 47, 446-450.	2.9	298
9	Phase stability in the Feâ€“Ni system: Investigation by first-principles calculations and atomistic simulations. Acta Materialia, 2005, 53, 4029-4041.	3.8	262
10	Tight-binding total-energy method for transition and noble metals. Physical Review B, 1994, 50, 14694-14697.	1.1	258
11	The AFLOW standard for high-throughput materials science calculations. Computational Materials Science, 2015, 108, 233-238.	1.4	244
12	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.	1.1	185
13	Calculated elastic and thermal properties of MGO at high pressures and temperatures. Journal of Geophysical Research, 1990, 95, 7055-7067.	3.3	154
14	The AFLOW Library of Crystallographic Prototypes: Part 1. Computational Materials Science, 2017, 136, S1-S828.	1.4	147
15	Electronic structure calculations of lead chalcogenides PbS, PbSe, PbTe. Journal of Physics and Chemistry of Solids, 2002, 63, 833-841.	1.9	143
16	New low-energy crystal structure for silicon. Physical Review Letters, 1991, 67, 715-718.	2.9	97
17	Beyond the Rigid-Ion Approximation with Spherically Symmetric Ions. Physical Review Letters, 1985, 54, 1940-1943.	2.9	85
18	Tight-binding study of stacking fault energies and the Rice criterion of ductility in the fcc metals. Physical Review B, 2000, 61, 4894-4897.	1.1	85

#	Article	IF	Citations
19	The AFLOW Library of Crystallographic Prototypes: Part 2. Computational Materials Science, 2019, 161, S1-S1011.	1.4	70
20	AFLOW-CHULL: Cloud-Oriented Platform for Autonomous Phase Stability Analysis. Journal of Chemical Information and Modeling, 2018, 58, 2477-2490.	2.5	69
21	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.	1.9	66
22	Phase stability of wÃ¼stite at high pressure from first-principles linearized augmented plane-wave calculations. Physical Review B, 1993, 47, 7720-7731.	1.1	56
23	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> anab initiohigh-throughput approach. Physical Review B, 2015, 91, .	1.1	54
24	Epitaxial Growth of Cubic and Hexagonal InN Thin Films via Plasma-Assisted Atomic Layer Epitaxy. Crystal Growth and Design, 2013, 13, 1485-1490.	1.4	45
25	All-electron first-principles supercell total-energy calculation of the vacancy formation energy in aluminium. Physica B: Condensed Matter, 1991, 172, 211-215.	1.3	44
26	Tetragonal Phase Transformation in Gold Nanowires. Journal of Engineering Materials and Technology, Transactions of the ASME, 2005, 127, 417-422.	0.8	44
27	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.	0.0	44
28	The Van der Waals interaction between an atom and a solid. Surface Science, 1980, 99, 553-569.	0.8	43
29	Application of a tight-binding total-energy method for Al, Ga, and In. Physical Review B, 1998, 57, R2013-R2016.	1.1	40
30	Ab InitioBased Tight-Binding Hamiltonian for the Dissociation of Molecules at Surfaces. Physical Review Letters, 1999, 82, 1209-1212.	2.9	36
31	Calculations of superconducting properties in yttrium and calcium under high pressure. Physical Review B, 2007, 75, .	1.1	32
32	First-principles calculation of the elastic moduli ofNi3Al. Physical Review B, 1991, 43, 1805-1807.	1.1	31
33	Absence of metastable states in strained monatomic cubic crystals. Physical Review B, 2004, 70, .	1.1	29
34	Interlayer surface relaxations and energies of fcc metal surfaces by a tight-binding method. Physical Review B, 2004, 70, .	1.1	29
35	Calculation of energy barriers for physically allowed lattice-invariant strains in aluminum and iridium. Physical Review B, 1991, 43, 9498-9502.	1.1	28
36	AFLOW-XtalFinder: a reliable choice to identify crystalline prototypes. Npj Computational Materials, 2021, 7, .	3.5	28

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37	Settling the matter of the role of vibrations in the stability of high-entropy carbides. Nature Communications, 2021, 12, 5747.	5.8	28
38	Active bialkali photocathodes on free-standing graphene substrates. Npj 2D Materials and Applications, 2017, 1, .	3.9	24
39	Theoretical confirmation of the experimental Raman spectra of the lower-order diamondoid molecule: cyclohexamantane (C26H30). Chemical Physics Letters, 2005, 403, 83-88.	1.2	21
40	Electronic structure and superconducting properties of lanthanum. Physical Review B, 2008, 78, .	1.1	20
41	Spherical self-consistent atomic deformation model for first-principles energy calculations in ionic crystalline solids. Physical Review B, 1996, 54, 7729-7736.	1.1	19
42	Occupation-number broadening schemes: Choice of â€œtemperatureâ€• Physical Review B, 2000, 61, 1654-1657.	1.1	19
43	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.	1.9	17
44	The AFLOW Library of Crystallographic Prototypes: Part 3. Computational Materials Science, 2021, 199, 110450.	1.4	16
45	Calculations of the superconducting properties of scandium under high pressure. Physical Review B, 2007, 76, .	1.1	15
46	Application of a tight-binding total-energy method for FeAl. Journal of Physics Condensed Matter, 2002, 14, 1895-1902.	0.7	13
47	Quantum theory of neutral-atom scattering at long range from solid cylinders. Physical Review A, 1980, 21, 1177-1184.	1.0	12
48	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
49	Tight-binding Hamiltonians for realistic electronic structure calculations. Physica B: Condensed Matter, 2001, 296, 129-137.	1.3	9
50	The AFLOW Fleet for Materials Discovery. , 2018, , 1-28.		9
51	Automated coordination corrected enthalpies with AFLOW-CCE. Physical Review Materials, 2021, 5, .	0.9	9
52	Consequences of zero-point motion to the radial distribution function of amorphous silicon. Journal of Physics Condensed Matter, 2004, 16, S5165-S5172.	0.7	7
53	A Brief History of Strukturbericht Symbols and Other Crystallographic Classification Schemes. Journal of Physics: Conference Series, 2019, 1290, 012016.	0.3	7
54	Tin-pest problem as a test of density functionals using high-throughput calculations. Physical Review Materials, 2021, 5, .	0.9	7

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55	Nearly metastable rhombohedral phases of bcc metals. Physical Review B, 2008, 77, .	1.1	4
56	Tight-Binding study of Boron structures. Journal of Physics and Chemistry of Solids, 2014, 75, 1106-1112.	1.9	4
57	The AFLOW Fleet for Materials Discovery. , 2020, , 1785-1812.		4
58	Understanding The Nb-Ti-A1 System: First Principles Calculations. Materials Research Society Symposia Proceedings, 1994, 364, 1265.	0.1	1
59	First-Principles Calculation of the Structure of Mercury. Materials Research Society Symposia Proceedings, 1995, 408, 383.	0.1	1
60	A Tight-Binding Hamiltonian for Band Structure and Carrier Transport in Graphene Nanoribbons. Materials Research Society Symposia Proceedings, 2007, 1057, 1.	0.1	1
61	Density functional study of the L10â€“Î±IrV transition in IrV and RhV. Journal of Alloys and Compounds, 2011, 509, 560-567.	2.8	1
62	Tight-Binding Total Energy Methods for Magnetic Materials and Multi-Element Systems. , 2005, , 275-305.		1
63	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
64	Theoretical studies of the vibrational properties of octahedrane (C12H12): A polyhedral caged hydrocarbon molecule. Journal of Chemical Physics, 2019, 150, 214304.	1.2	0
65	The AFLOW Fleet for Materials Discovery. , 2019, , 1-28.		0