John A Moriarty

List of Publications by Year in descending order

83 papers	5,432 citations	87886 38 h-index	79691 73 g-index
84 all docs	84 docs citations	84 times ranked	2225 citing authors

#	Article	IF	Citations
1	Local volume effects in the generalized pseudopotential theory. Physical Review B, 2019, 99, .	3.2	2
2	Polymorphism and melt in high-pressure tantalum. II. Orthorhombic phases. Physical Review B, 2018, 98, .	3.2	4
3	Efficient wide-range calculation of free energies in solids and liquids using reversible-scaling molecular dynamics. Physical Review B, 2014, 90, .	3.2	9
4	Polymorphism and melt in high-pressure tantalum. Physical Review B, 2012, 86, .	3.2	23
5	Quantum-Mechanical Interatomic Potentials with Electron Temperature for Strong-Coupling Transition Metals. Physical Review Letters, 2012, 108, 036401.	7.8	21
6	High-Pressureâ€"High-Temperature Polymorphism in Ta: Resolving an Ongoing Experimental Controversy. Physical Review Letters, 2010, 104, 255702.	7.8	78
7	Chapter 92 Dislocations and Plasticity in bcc Transition Metals at High Pressure. Dislocations in Solids, 2010, , 1-46.	1.6	29
8	Generalized pseudopotential theory of d-band metals. International Journal of Quantum Chemistry, 2009, 24, 541-554.	2.0	0
9	Quantum molecular dynamics simulations of uranium at high pressure and temperature. Physical Review B, 2008, 78, .	3.2	32
10	First-principles thermoelasticity of transition metals at high pressure: Tantalum prototype in the quasiharmonic limit. Physical Review B, 2006, 74, .	3.2	53
11	Robust quantum-based interatomic potentials for multiscale modeling in transition metals. Journal of Materials Research, 2006, 21, 563-573.	2.6	46
12	High-pressure tailored compression: Controlled thermodynamic paths. Journal of Applied Physics, 2006, 100, 023508.	2.5	37
13	Bridging the Gap Between Quantum Mechanics and Large-Scale Atomistic Simulation. , 2005, , 2737-2747.		0
14	Specifically Prescribed Dynamic Thermodynamic Paths and Resolidification Experiments. AIP Conference Proceedings, 2004, , .	0.4	14
15	PLEIADES: a subpicosecond Thomson x-ray source for ultrafast materials probing. , 2003, , .		0
16	The rigid-body displacement observed at the â^ = 5, (310)-[001] symmetric tilt grain boundary in central transition bcc metals. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2002, 82, 1573-1594.	0.6	3
17	Quantum-based atomistic simulation of materials properties in transition metals. Journal of Physics Condensed Matter, 2002, 14, 2825-2857.	1.8	147
18	Atomistic simulations of dislocations and defects. Journal of Computer-Aided Materials Design, 2002, 9, 99-132.	0.7	60

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19	Accurate atomistic simulation of (a/2) ã€ˆ111ã€‰ screw dislocations and other defects in bcc tantalum. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2001, 81, 1355-1385.	0.6	110
20	Transition-metal interactions in aluminum-rich intermetallics. Physical Review B, 2001, 64, .	3.2	25
21	Multiscale Modeling of Dislocation Processes in Bcc Tantalum: Bridging Atomistic and Mesoscale Simulations. Materials Research Society Symposia Proceedings, 2000, 653, 1.	0.1	1
22	Atomic structure of the Ïƒ5 (310)/[001] symmetric tilt grain boundary in tantalum. Scripta Materialia, 2000, 43, 659-664.	5.2	23
23	Multiscale Modeling of Dislocation Processes in Bcc Tantalum: Bridging Atomistic and Mesoscale Simulations. Materials Research Society Symposia Proceedings, 2000, 653, .	0.1	0
24	First-principles interatomic potentials for transition-metal aluminides. III. Extension to ternary phase diagrams. Physical Review B, 2000, 62, 3648-3657.	3.2	39
25	First-principles formation energies of monovacancies in bcc transition metals. Physical Review B, 2000, 61, 2579-2586.	3.2	91
26	Symmetrical tilt grain boundaries in bcc transition metals: Comparison of semiempirical with ab-initio total-energy calculations. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2000, 80, 2405-2423.	0.6	34
27	Atomistic Simulations for Multiscale Modeling in bcc Metals. Journal of Engineering Materials and Technology, Transactions of the ASME, 1999, 121, 120-125.	1.4	26
28	Ab initiothermoelasticity of magnesium. Physical Review B, 1999, 59, 3427-3433.	3.2	27
29	Atomic structure of the Î£5 (310)/[001] symmetric tilt grain boundary in molybdenum. Acta Materialia, 1999, 47, 3977-3985.	7.9	38
30	Electronic Effects on Grain Boundary Structure in Bcc Metals. Materials Research Society Symposia Proceedings, 1999, 589, 347.	0.1	0
31	Accurate atomistic simulations of the Peierls barrier and kink-pair formation energy for ã€ˆ111ã€‰ screw dislocations in bcc Mo. Computational Materials Science, 1998, 9, 348-356.	3.0	68
32	First-principles interatomic potentials for transition-metal aluminides. II. Application to Al-Co and Al-Ni phase diagrams. Physical Review B, 1998, 58, 8967-8979.	3.2	31
33	First-principles theory of Ta up to 10 Mbar pressure: Structural and mechanical properties. Physical Review B, 1998, 57, 10340-10350.	3.2	96
34	First-principles interatomic potentials for transition-metal aluminides: Theory and trends across the3dseries. Physical Review B, 1997, 56, 7905-7917.	3.2	83
35	Equation of state of beryllium at shock pressures of 0.4â€“1.1 TPa (4â€“11 Mbar). Journal of Applied Physics, 1997, 82, 2225-2227.	2.5	36
36	First-principles theory of iron up to earth-core pressures: Structural, vibrational, and elastic properties. Physical Review B, 1996, 53, 14063-14072.	3.2	240

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37	EAM potential for magnesium from quantum mechanical forces. Modelling and Simulation in Materials Science and Engineering, 1996, 4, 293-303.	2.0	264
38	Atomistic simulation of point defects and dislocations in bcc transition metals from first principles. Journal of Computer-Aided Materials Design, 1996, 3, 245-252.	0.7	2
39	Atomistic simulation of ideal shear strength, point defects, and screw dislocations in bcc transition metals: Mo as a prototype. Physical Review B, 1996, 54, 6941-6951.	3.2	139
40	First-principles equations of state for Al, Cu, Mo, and Pb to ultrahigh pressures. High Pressure Research, 1995, 13, 343-365.	1.2	22
41	First-principles temperature-pressure phase diagram of magnesium. Physical Review B, 1995, 51, 5609-5616.	3.2	49
42	Angular forces and melting in bcc transition metals: A case study of molybdenum. Physical Review B, 1994, 49, 12431-12445.	3.2	118
43	Phase diagram and thermodynamic properties of solid magnesium in the quasiharmonic approximation. Physical Review B, 1993, 48, 13253-13260.	3.2	67
44	High-pressure melting temperatures of uranium: Laser-heating experiments and theoretical calculations. Physical Review B, 1993, 48, 15529-15534.	3.2	23
45	Ultrahigh-pressure structural phase transitions in Cr, Mo, and W. Physical Review B, 1992, 45, 2004-2014.	3.2	89
46	Equation of state of Al, Cu, Mo, and Pb at shock pressures up to 2.4 TPa (24 Mbar). Journal of Applied Physics, 1991, 69, 2981-2986.	2.5	146
47	First-principles interatomic potentials for transition-metal surfaces. Physical Review Letters, 1991, 66, 3036-3039.	7.8	82
48	First-Principles Interatomic Potentials for Transition Metals and Their Surfaces. Materials Research Society Symposia Proceedings, 1990, 193, 9.	0.1	0
49	Analytic representation of multi-ion interatomic potentials in transition metals. Physical Review B, 1990, 42, 1609-1628.	3.2	176
50	The equation of state of platinum to 660 GPa (6.6 Mbar). Journal of Applied Physics, 1989, 66, 2962-2967.	2.5	498
51	Acoustic Velocities and Phase Transitions in Molybdenum under Strong Shock Compression. Physical Review Letters, 1989, 62, 637-640.	7.8	197
52	High-pressure structural phase stability in Hg TO 1 TPa (10 Mbar). Physics Letters, Section A: General, Atomic and Solid State Physics, 1988, 131, 41-46.	2.1	39
53	Metals physics at ultrahigh pressure: Aluminum, copper, and lead as prototypes. Physical Review Letters, 1988, 60, 1414-1417.	7.8	220
54	Density-functional formulation of the generalized pseudopotential theory. III. Transition-metal interatomic potentials. Physical Review B, 1988, 38, 3199-3231.	3.2	189

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55	First-principles phonon spectrum in bcc Ba: Three-ion forces and transition-metal behavior. Physical Review B, 1986, 34, 6738-6745.	3.2	39
56	High-Pressure Ion-Thermal Properties of Metals from AB Initio Interatomic Potentials. , 1986, , 101-106.		30
57	Electronic structure of silicon superlattices. Superlattices and Microstructures, 1985, 1, 209-215.	3.1	3
58	First-Principles Interatomic Potentials in Transition Metals. Physical Review Letters, 1985, 55, 1502-1505.	7.8	32
59	Electronic structure and impurity-limited electron mobility of silicon superlattices. Physical Review B, 1985, 32, 1027-1036.	3.2	17
60	Theoretical study of the aluminum melting curve to very high pressure. Physical Review B, 1984, 30, 578-588.	3.2	107
61	Structural phase stability in third-period simple metals. Physical Review B, 1983, 27, 3235-3251.	3.2	196
62	Theory of silicon superlattices: Electronic structure and enhanced mobility. Journal of Applied Physics, 1983, 54, 1892-1902.	2.5	56
63	First-principles phonon spectra in Ca and Sr. Physical Review B, 1983, 28, 4818-4821.	3.2	24
64	Density-functional formulation of the generalized pseudopotential theory. II. Physical Review B, 1982, 26, 1754-1780.	3.2	117
65	High-Pressure Structural Phase Transitions in Na, Mg, and Al. Physical Review Letters, 1982, 48, 809-812.	7.8	133
66	Smallâ€signal ac response of dielectric materials containing static spaceâ€charge fields: Application to ionic conductors and MIS structures. Journal of Applied Physics, 1981, 52, 3413-3427.	2.5	2
67	Si and GaAs photocapacitive MIS infrared detectors. Journal of Applied Physics, 1980, 51, 2137.	2.5	21
68	Improved characterization of the Siâ€SiO2interface. Applied Physics Letters, 1980, 36, 991-993.	3.3	8
69	Simplified local-density theory of the cohesive energy of metals. Physical Review B, 1979, 19, 609-619.	3.2	27
70	LaF3insulators for MIS structures. Applied Physics Letters, 1979, 34, 799-801.	3.3	11
71	The small-core approximation and structural phase stability in metals. Solid State Communications, 1979, 31, 881-884.	1.9	3
72	Modified latticeâ€statics approach to dislocation calculations. II. Application. Journal of Applied Physics, 1978, 49, 3960-3966.	2.5	6

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73	Photocapacitive MIS infrared detectors. Applied Physics Letters, 1978, 32, 713-715.	3.3	8
74	Density-functional formulation of the generalized pseudopotential theory. Physical Review B, 1977, 16, 2537-2555.	3.2	85
75	Two-electron bond-orbital model. II. Physical Review B, 1976, 14, 2539-2558.	3.2	14
76	Equivalence of resonance and tight binding descriptions of the d band in transition metals. Journal of Physics F: Metal Physics, 1975, 5, 873-882.	1.6	19
77	Two-electron bond-orbital model I. Physical Review B, 1975, 12, 5395-5406.	3.2	12
78	Zero-order pseudoatoms and the generalized pseudopotential theory. Physical Review B, 1974, 10, 3075-3091.	3.2	59
79	Hybridization and the fcc-bcc Phase Transitions in Calcium and Strontium. Physical Review B, 1973, 8, 1338-1345.	3.2	60
80	LocalizeddStates for Pseudopotential Calculations: Application to the Alkaline-Earth Metals. Physical Review B, 1972, 6, 4445-4458.	3.2	73
81	Total Energy of Copper, Silver, and Gold. Physical Review B, 1972, 6, 1239-1252.	3.2	177
82	Pseudo Green's Functions and the Pseudopotential Theory ofd-Band Metals. Physical Review B, 1972, 5, 2066-2081.	3.2	86
83	Pseudopotential Form Factors for Copper, Silver, and Gold. Physical Review B, 1970, 1, 1363-1370.	3.2	161