Anthony Thomas Paxton

List of Publications by Year
in descending order

81 papers	9,329 citations	185998 28 h-index	64668 79 g-index
82 all docs	82 docs citations	82 times ranked	8498 citing authors

#	Article	IF	Citations
1	High-precision sampling for Brillouin-zone integration in metals. Physical Review B, 1989, 40, 3616-3621.	1.1	6,201
2	A stabilization mechanism of zirconia based on oxygen vacancies only. Acta Materialia, 2002, 50, 5171-5178.	3.8	330
3	Structural energy-volume relations in first-row transition metals. Physical Review B, 1990, 41, 8127-8138.	1.1	204
4	Chain-Fragment Doping and the Phase Diagram ofYBa2Cu3O7â^'x. Physical Review Letters, 1988, 60, 2685-2688.	2.9	189
5	Bismuth embrittlement of copper is an atomic size effect. Nature, 2004, 432, 1008-1011.	13.7	174
6	SrTiO3(001)(2Ã—1)reconstructions:â€ƒFirst-principles calculations of surface energy and atomic structure compared with scanning tunneling microscopy images. Physical Review B, 2004, 70, .	1.1	154
7	Crystal Structures of Zirconia from First Principles and Self-Consistent Tight Binding. Physical Review Letters, 1998, 81, 5149-5152.	2.9	132
8	Structural and chemical embrittlement of grain boundaries by impurities: A general theory and first-principles calculations for copper. Physical Review B, 2006, 74, .	1.1	127
9	A quantum mechanical calculation of the theoretical strength of metals. Philosophical Magazine Letters, 1991, 63, 267-274.	0.5	116
10	Relative energetics and structural properties of zirconia using a self-consistent tight-binding model. Physical Review B, 2000, 61, 6617-6630.	1.1	82
11	Electronic structure and phase stability study in the Ni-Ti system. Physical Review B, 1995, 52, 15176-15190.	1.1	76
12	Evidences of transitory metastable phases in refractory metals solidified from highly undercooled liquids in a drop tube. Physical Review Letters, 1993, 70, 1469-1472.	2.9	75
13	First-principles determination of the Ni-Al phase diagram. Journal of Physics Condensed Matter, 1992, 4, 945-959.	0.7	73
14	The near-edge structure in energy-loss spectroscopy: many-electron and magnetic effects in transition metal nitrides and carbides. Journal of Physics Condensed Matter, 2000, 12, 729-750.	0.7	71
15	A bandstructure view of the Humeâ€Rothery electron phases. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 1997, 453, 1493-1514.	1.0	66
16	Boron in copper: A perfect misfit in the bulk and cohesion enhancer at a grain boundary. Physical Review B, 2008, 77, .	1.1	65
17	Interatomic forces in transition metals. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1988, 58, 143-163.	0.8	63
18	A tight-binding study of grain boundaries in silicon. Acta Metallurgica, 1989, 37, 1693-1715.	2.1	63

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19	A simple theoretical approach to grain boundaries in silicon. Journal of Physics C: Solid State Physics, 1988, 21, L481-L488.	1.5	62
20	Effect of relaxation on the oxygenK-edge electron energy-loss near-edge structure in yttria-stabilized zirconia. Physical Review B, 2000, 62, 14728-14735.	1.1	53
21	Electron energy-loss near-edge shape as a probe to investigate the stabilization of yttria-stabilized zirconia. Physical Review B, 2002, 65, .	1.1	52
22	Structural stability of silicon in tight-binding models. Journal of Physics C: Solid State Physics, 1987, 20, L263-L269.	1.5	47
23	Defects in ZnTe, CdTe, and HgTe: Total energy calculations. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1990, 8, 1103-1107.	0.9	44
24	A comparison of methods for calculating tight-binding bond energies. Journal of Physics F: Metal Physics, 1988, 18, 693-718.	1.6	40
25	Electronic structure and total energy of interstitial hydrogen in iron: Tight-binding models. Physical Review B, 2010, 82, .	1.1	40
26	Magnetic tight binding and the iron-chromium enthalpy anomaly. Physical Review B, 2008, 77, .	1.1	39
27	Hydrogen embrittlement I. Analysis of hydrogen-enhanced localized plasticity: Effect of hydrogen on the velocity of screw dislocations in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math>-Fe. Physical Review Materials, 2017, 1, .	0.9	39
28	Density functional theory calculations of iron - vanadium carbide interfaces and the effect of hydrogen. International Journal of Hydrogen Energy, 2020, 45, 2382-2389.	3.8	33
29	Hydrogen Diffusion and Trapping in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Iron: The Role of Quantum and Anharmonic Fluctuations. Physical Review Letters, 2018, 120, 225901.	2.9	26
30	Atomistic studies of interactions between the dominant lattice dislocations and Î³/Î³-lamellar boundaries in lamellar Î³-TiAl. Acta Materialia, 2009, 57, 3349-3366.	3.8	25
31	Analysis of a carbon dimer bound to a vacancy in iron using density functional theory and a tight binding model. Physical Review B, 2013, 87, .	1.1	25
32	Stability of Sr adatom model structures for SrTiO3(001) surface reconstructions. Journal of Physics Condensed Matter, 2005, 17, L223-L230.	0.7	24
33	Atomic structure of metallic interfaces. Journal Physics D: Applied Physics, 1996, 29, 1689-1698.	1.3	23
34	Atomistic study of ordinary screw dislocations in single-phase and lamellar Î³-TiAl. Philosophical Magazine, 2007, 87, 1795-1809.	0.7	23
35	On the phase stability of transition metal trialuminide compounds. Intermetallics, 1995, 3, 9-14.	1.8	21
36	Origin of the Modulated Phase in Copper-Gold Alloys. Physical Review Letters, 1997, 78, 270-273.	2.9	21

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37	Nonconservative current-induced forces: A physical interpretation. Beilstein Journal of Nanotechnology, 2011, 2, 727-733.	1.5	21
38	Quantum and isotope effects on hydrogen diffusion, trapping and escape in iron. Acta Materialia, 2016, 103, 71-76.	3.8	21
39	Theoretical evaluation of the role of crystal defects on local equilibrium and effective diffusivity of hydrogen in iron. Materials Science and Technology, 2017, 33, 1505-1514.	0.8	21
40	Stabilizing Role of Itinerant Ferromagnetism in Intergranular Cohesion in Iron. Physical Review Letters, 1998, 81, 2998-3001.	2.9	19
41	Fully quantum mechanical calculation of the diffusivity of hydrogen in iron using the tight-binding approximation and path integral theory. Physical Review B, 2013, 88, .	1.1	17
42	Al3Ruâ€”A ductile trialuminide?. Scripta Metallurgica Et Materialia, 1992, 26, 529-533.	1.0	16
43	How dislocations affect transport. Journal of Electronic Materials, 1995, 24, 525-532.	1.0	16
44	From quantum mechanics to physical metallurgy of steels. Materials Science and Technology, 2014, 30, 1063-1070.	0.8	16
45	Electronic structure of ordered and disordered Pd3Fe. Journal of Magnetism and Magnetic Materials, 1990, 87, 97-105.	1.0	15
46	The challenges of hydrogen and metals. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20170198.	1.6	15
47	The influence of hydrogen on plasticity in pure ironâ€”theory and experiment. Scientific Reports, 2020, 10, 10209.	1.6	15
48	A first-principles phase stability study on the Au-Ni system. Journal of Physics Condensed Matter, 1994, 6, L47-L52.	0.7	14
49	Hydrogen embrittlement II. Analysis of hydrogen-enhanced decohesion across (111) planes in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math> -Fe. Physical Review Materials, 2017, 1, .	0.9	14
50	Electronic structure and total-energy calculations forNiTi2-type structures. Physical Review B, 1993, 48, 14801-14808.	1.1	13
51	The impossibility of pseudotwinning in B2 alloys. Acta Metallurgica Et Materialia, 1995, 43, 2133-2136.	1.9	13
52	Bandstructure approach to near edge structure. Journal of Microscopy, 2003, 210, 35-44.	0.8	13
53	Phase stability in silicon from the point of view of the bond order. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1988, 58, 603-621.	0.6	12
54	Material Effects on Stress-Induced Defect Generation in Trenched Silicon-on-Insulator Structures. Journal of the Electrochemical Society, 2001, 148, G649.	1.3	11

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55	Theory of the near K-edge structure in electron energy loss spectroscopy. Journal of Electron Spectroscopy and Related Phenomena, 2005, 143, 51-64.	0.8	11
56	A crystal plasticity assessment of normally-loaded sliding contact in rough surfaces and galling. Journal of the Mechanics and Physics of Solids, 2018, 121, 517-542.	2.3	11
57	A tight binding model for water. Journal of Chemical Physics, 2011, 134, 044130.	1.2	10
58	Embrittlement of an elasto-plastic medium by an inclusion. International Journal of Fracture, 2019, 216, 87-100.	1.1	9
59	Recent Advances in Non Self-Consistent Total Energy Calculations in Alloys. Materials Research Society Symposia Proceedings, 1990, 186, 107.	0.1	8
60	Universal tight binding model for chemical reactions in solution and at surfaces. I. Organic molecules. Journal of Chemical Physics, 2014, 141, 044503.	1.2	8
61	Deformation twinning in the intermetallic compound Cu2Sb. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1985, 52, 573-579.	0.8	7
62	On the solvation of L-aspartic acid. Molecular Physics, 2004, 102, 953-958.	0.8	7
63	Microscopic Origin of Channeled Flow in Lamellar Titanium Aluminide. Physical Review Letters, 2010, 104, 225502.	2.9	7
64	Is the pinning of ordinary dislocations in Î³-TiAl intrinsic or extrinsic in nature? A combined atomistic and kinetic Monte Carlo approach. Acta Materialia, 2011, 59, 1281-1290.	3.8	7
65	An ignition key for atomic-scale engines. Journal of Physics Condensed Matter, 2012, 24, 402203.	0.7	7
66	Effect of applied strain on the interaction between hydrogen atoms and 12âŸ¨111âŸ© screw dislocations in Î±-iron. International Journal of Hydrogen Energy, 2020, 45, 20069-20079.	3.8	7
67	Effect of hydrogen on vacancy diffusion. Physical Review Materials, 2020, 4, .	0.9	6
68	Structural stability of NiTi2intermetallic compounds. Journal of Physics Condensed Matter, 1993, 5, 9087-9098.	0.7	5
69	Self-Consistent Tight-Binding Approximation Including Polarisable Ions. Materials Research Society Symposia Proceedings, 1997, 491, 265.	0.1	5
70	Ring currents in azulene. Chemical Physics Letters, 2009, 483, 154-158.	1.2	5
71	Universal tight binding model for chemical reactions in solution and at surfaces. II. Water. Journal of Chemical Physics, 2014, 141, 044504.	1.2	5
72	Hydrogen suppression of dislocation cell formation in micro and nano indentation of pure iron single crystals. Scripta Materialia, 2021, 194, 113683.	2.6	5

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73	Universal tight binding model for chemical reactions in solution and at surfaces. III. Stoichiometric and reduced surfaces of titania and the adsorption of water. Journal of Chemical Physics, 2014, 141, 044505.	1.2	4
74	Influence of hydrogen core force shielding on dislocation junctions in iron. Physical Review Materials, 2020, 4, .	0.9	4
75	Effects of calcium on planar fault energies in ternary magnesium alloys. Physical Review Materials, 2019, 3, .	0.9	3
76	Electronic structure and stability of the transition metal oxide Ni2Ti4O. Journal of Physics Condensed Matter, 1994, 6, 2861-2868.	0.7	2
77	Local volume effects in the generalized pseudopotential theory. Physical Review B, 2019, 99, .	1.1	2
78	The use of XANES and ELNES for the Characterisation of Stabilised Zirconia. Materials Research Society Symposia Proceedings, 2001, 699, 821.	0.1	1
79	Interatomic Forces and Bond Energies in the Tight Binding Approximation. , 1989, , 327-345.		1
80	Ising-like models for stacking faults in a free electron metal. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2020, 476, 20200319.	1.0	1
81	Dynamic strain aging and the role of the Cottrell atmosphere. Physical Review Materials, 2022, 6, .	0.9	1