Covalent effects in the effective-medium theory of cher solution in the3dmetals

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Citation Report

#	Article	IF	CITATIONS
1	Electronic structure of transition metal compounds; ground-state properties of the 3d-monoxides in the atomic sphere approximation. Pure and Applied Chemistry, 1980, 52, 93-118.	0.9	232
2	Interaction of Hydrogen with Defects in Metals: Interplay between Theory and Experiment. Physical Review Letters, 1982, 49, 1420-1423.	2.9	110
3	Cluster calculations of intermediate states in the catalyzed conversion of CH3OH to CH2O on a Cu(100) surface. Journal of Catalysis, 1983, 84, 288-296.	3.1	11
4	Theoretical studies of molecular adsorption on metal surfaces. International Journal of Quantum Chemistry, 1983, 23, 1083-1090.	1.0	2
5	Theoretical aspects of adsorption and heterogeneous catalysis. Vacuum, 1983, 33, 639-649.	1.6	23
6	Potentials for atom-surface scattering. Surface Science, 1983, 126, 675-680.	0.8	24
7	Semiempirical, Quantum Mechanical Calculation of Hydrogen Embrittlement in Metals. Physical Review Letters, 1983, 50, 1285-1288.	2.9	2,414
8	Hydrogen adsorption on a CuNi(111) surface. Journal of Physics C: Solid State Physics, 1983, 16, 3641-3647.	1.5	3
9	Interaction of helium with a metal surface. Physical Review B, 1983, 27, 4612-4616.	1.1	129
10	Quantum Motion of Chemisorbed Hydrogen on Ni Surfaces. Physical Review Letters, 1983, 51, 1081-1084.	2.9	156
11	Atoms embedded in an electron gas: Phase shifts and cross sections. Physical Review B, 1983, 27, 6121-6128.	1.1	211
12	Application of simple model theories to thermodynamic properties of liquid transition metals. Journal of Physics F: Metal Physics, 1984, 14, L15-L20.	1.6	48
13	Muon states in uniaxially strained iron. Physical Review B, 1984, 29, 4170-4172.	1.1	4
14	Defect trapping of ionâ€implanted deuterium in copper. Journal of Applied Physics, 1984, 56, 3384-3393.	1.1	70
15	Electronically induced trapping of hydrogen by impurities in niobium. Physical Review B, 1984, 30, 1065-1068.	1.1	21
16	Muon states in metals: Recent progress. Hyperfine Interactions, 1984, 17, 167-176.	0.2	4
17	Interaction of deuterium with lattice defects in nickel. Nuclear Instruments & Methods in Physics Research B, 1984, 4, 374-387.	0.6	31
18	Theory nof chemisorption and heterogeneous catalysis. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1984, 127, 193-202.	0.9	10

#	Article	IF	CITATIONS
19	Hydrogen in metals: Quantum aspects. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1984, 127, 417-421.	0.9	2
20	Hydrogen adsorption on metal surfaces. Surface Science, 1984, 136, 59-81.	0.8	400
21	Metal-support interactions in heterogeneous catalysis. Surface Science, 1984, 138, 84-94.	0.8	70
22	Heat of formation and band structure of binary and ternary metal hydrides. Physical Review B, 1984, 30, 4372-4381.	1.1	136
23	Site preference of interstitial hydrogen in metals. Journal of the Less Common Metals, 1984, 101, 1-16.	0.9	65
24	Positive muon knight shift studies and the electronic structure of hydrogen in metals. Journal of the Less Common Metals, 1984, 101, 97-113.	0.9	16
25	Role of multi-adatom interactions in the formation of ordered structures on metal surfaces: Application to H/Fe(110). Surface Science, 1984, 139, 491-504.	0.8	29
26	The binding of hydrogen to a Pd(111) surface. Surface Science, 1984, 148, 237-251.	0.8	19
27	Microscopic model for the poisoning and promotion of adsorption rates by electronegative and electropositive atoms. Surface Science, 1984, 137, 65-78.	0.8	320
28	A molecular orbital study of hydrogen atoms implanted in titanium metal clusters. Surface Science, 1984, 137, 181-196.	0.8	4
29	Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. Physical Review B, 1984, 29, 6443-6453.	1.1	6,059
30	Theory of hydrogen and helium impurities in metals. Physical Review B, 1984, 29, 5382-5397.	1.1	146
31	Atomic relaxation and electronic structure of dilute alloys in the tight-binding approximation. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1985, 52, 971-985.	0.6	5
32	Surface states and the local electronic structure at surfaces. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1985, 51, 223-241.	0.6	59
33	The low-temperature diffusion of Hydrogen through annealed, quenched and aged gold. Journal of Physics and Chemistry of Solids, 1985, 46, 1393-1396.	1.9	9
34	Embedded cluster model studies of impurities at metal surfaces. Progress in Surface Science, 1985, 18, 59-188.	3.8	23
35	Oxygen chemisorption and incorporation on transition metal surfaces. Surface Science Letters, 1985, 152-153, A141.	0.1	0
36	On the electronic structure of the light rare earth hydrides. European Physical Journal B, 1985, 61, 113-128.	0.6	48

#	Article	IF	CITATIONS
37	Interaction of hydrogen with defects in metals. Nuclear Instruments & Methods in Physics Research B, 1985, 7-8, 55-66.	0.6	78
38	The diffusivity of hydrogen in the noble metals at low temperature. Acta Metallurgica, 1985, 33, 1979-1985.	2.1	36
39	Adsorbate-Surface Interactions. Springer Series in Solid-state Sciences, 1985, , 94-103.	0.3	1
40	Energy of immersing a He, Ne, or Ar atom orH2molecule into a low-density electron gas. Physical Review B, 1985, 31, 727-729.	1.1	47
41	Model adsorption potentials for He and Ne on graphite. Physical Review B, 1985, 32, 6989-6992.	1.1	38
42	Excitation of Hydrogen Motion inside a Nickel Vacancy. Physical Review Letters, 1985, 55, 852-855.	2.9	29
43	Local-orbital analysis of oxygen-oxygen interaction on nickel (001) from self-consistent electronic structure. Physical Review B, 1985, 32, 7641-7645.	1.1	5
44	Electronic structure of interstitial impurities near surfaces. Physical Review B, 1985, 31, 3398-3404.	1.1	11
45	Electrostatic adsorbate-adsorbate interactions: The poisoning and promotion of the molecular adsorption reaction. Surface Science, 1985, 150, 24-38.	0.8	371
46	Indirect electronic interaction between hydrogen atoms adsorbed on metals. Surface Science, 1985, 159, 443-465.	0.8	57
47	Oxygen chemisorption and incorporation on transition metal surfaces. Surface Science, 1985, 152-153, 660-683.	0.8	71
48	UPS spectra of H2O, CH3OH and C5H9OH adsorbed onto Cu(111)/Na and Na(cp). Surface Science, 1985, 160, 599-617.	0.8	38
49	The lattice response to embedding of helium impurities in BCC metals. Journal of Physics F: Metal Physics, 1985, 15, 2409-2420.	1.6	11
50	Ordered hydrogen overlayers on metal surfaces. Physical Review B, 1986, 33, 8136-8145.	1.1	45
51	Modification of Cu-H bonding near a Ru(0001) surface. Surface Science, 1986, 173, L582-L589.	0.8	20
52	Calculation of helium diffraction from metal surfaces. Surface Science, 1986, 169, 299-316.	0.8	13
53	Calculations of the energetics and structure of Pt(110) reconstruction using the embedded atom method. Surface Science, 1986, 166, L161-L169.	0.8	118
54	A theoretical study of carbon chemisorption on nickel surfaces. Surface Science, 1986, 166, 539-553.	0.8	23

ARTICLE IF CITATIONS # Calculated Adsorption Properties of Be on Metals. Studies in Surface Science and Catalysis, 1986, 26, 55 1.5 0 319-332. The diffusivity of hydrogen in aluminum. Acta Metallurgica, 1986, 34, 1091-1095. 2.1 93 57 Modification of Cu-H bonding near a Ru(0001) surface. Surface Science Letters, 1986, 173, L582-L589. 0.1 0 Calculations of the energetics and structure of Pt(110) reconstruction using the embedded atom 0.1 method. Surface Science Letters, 1986, 166, L161-L168. Calculated adsorption properties of be on metals. Journal of Electron Spectroscopy and Related 59 0.8 4 Phenomena, 1986, 39, 319-332. The diffusivity of hydrogen through solid solutions of palladium with the transition metals. Journal of Physics and Chemistry of Solids, 1986, 47, 225-229. Commentary on local densities of states, surface bonds and rate processes. Philosophical 61 1.3 3 Transactions of the Royal Society A, 1986, 318, 135-139. Interatomic interactions in solids: An effective-medium approach. Physical Review B, 1986, 34, 8486-8495. 1.1 54 Trends in hydrogen heats of solution and vacancy trapping energies in transition metals. Journal of 63 1.6 101 Physics F: Metal Physics, 1986, 16, 1161-1171. Theoretical Analysis of Vibrational Modes of an OH Molecule Adsorbed on a Transition Metal Surface. 64 1.2 Physica Scripta, 1987, 35, 181-184. Bond weakening by hydrogen in transition metals. Physical Review B, 1987, 35, 1076-1081. 65 1.1 14 Model adsorption potentials of rare gases on boron nitride. Physical Review B, 1987, 36, 7576-7579. 1.1 Calculation of the barrier for oxygen incorporation into metal and metal-oxide surfaces. Physical 67 1.1 21 Review B, 1987, 36, 4982-4989. Hydrogen and deuterium decoration of In-vacancy complexes in nickel. Physical Review B, 1987, 35, 1.1 6059-6063. 69 Hydrogen in transition metals., 1987, , 146-163. 1 Surface effects controlling electron-stimulated oxidation of silicon. Philosophical Magazine Letters, 1987, 55, 53-58. Theoretical aspects of surface reactions. Surface Science, 1987, 189-190, 91-105. 71 0.8 71 Interatomic interactions in the effective-medium theory. Physical Review B, 1987, 35, 7423-7442. 1.1 868

#	Article	IF	CITATIONS
73	Theory of subsurface occupation, ordered structures, and order-disorder transitions for hydrogen on Pd(111). Physical Review B, 1987, 35, 2128-2136.	1.1	98
74	Electronic structure and total energy calculations for transition metal hydrides. Journal of the Less Common Metals, 1987, 130, 249-259.	0.9	34
75	Theory of hydrogen interaction with metals. Journal of the Less Common Metals, 1987, 130, 475-490.	0.9	155
76	Theoretical study of the H-induced (1 × 2)-reconstruction at the Ni(110) surface. Surface Science, 1987, 179, L91-L101.	0.8	8
77	Theory of H bonding and vibration on Ru(0001). Surface Science, 1987, 179, 153-162.	0.8	42
78	Theoretical descriptions of atomic and molecular chemisorption on metals. Progress in Surface Science, 1987, 25, 191-210.	3.8	5
79	Multiple hydrogen occupancy of vacancies in Fe. Journal of Applied Physics, 1987, 61, 1788-1794.	1.1	104
80	Dynamics of Atoms in Low-Symmetry Systems. Physica Scripta, 1987, T19A, 320-325.	1.2	3
81	The thermodynamics of dilute solutions of hydrogen in palladium and its substitutional alloys. Acta Metallurgica, 1987, 35, 197-225.	2.1	59
82	The Thermodynamic Properties of Liquid Transition and Rareâ€Earth Metals Based on CHS Model. Physica Status Solidi (B): Basic Research, 1987, 144, 557-564.	0.7	8
83	Interaction of hydrogen with defects in metals. Soviet Atomic Energy, 1987, 62, 131-142.	0.1	5
84	Dynamic embrittlement of boron-doped Ni3Al alloys at 600°C. Acta Metallurgica, 1987, 35, 643-649.	2.1	162
85	Theoretical study of the H-induced (1×2)-reconstruction at the Ni(110) surface. Surface Science Letters, 1987, 179, L91-L101.	0.1	0
86	Electronic structure and bonding in metal hydrides, studied with photoelectron spectroscopy. European Physical Journal B, 1987, 66, 441-458.	0.6	29
87	Interaction of hydrogen with solid surfaces. Surface Science Reports, 1988, 9, 1-163.	3.8	1,051
88	The solubility of hydrogen in liquid binary Al-Li alloys. Metallurgical and Materials Transactions B - Process Metallurgy and Materials Processing Science, 1988, 19, 227-232.	0.5	26
89	Heat of formation models. Topics in Applied Physics, 1988, , 219-284.	0.4	97
90	The tight-binding bond model. Journal of Physics C: Solid State Physics, 1988, 21, 35-66.	1.5	422

#	Article	IF	Citations
91	Interatomic forces in transition metals. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1988, 58, 143-163.	0.8	63
92	Many-body embedded-atom potential for describing the energy and angular distributions of Rh atoms desorbed from ion-bombarded Rh{111}. Physical Review B, 1988, 37, 7197-7204.	1.1	108
93	Thermodynamics of liquid metals based on charged hard sphere (CHS) model. Physica Scripta, 1988, 37, 762-767.	1.2	17
94	The influence of coadsorbed K on the electronic energy levels of chemisorbed CO. Surface Science, 1988, 206, L864-L870.	0.8	18
95	Electronic properties. Topics in Applied Physics, 1988, , 139-217.	0.4	32
96	Interaction of an Aromatic Molecule with a Surface. Materials Research Society Symposia Proceedings, 1988, 131, 611.	0.1	0
97	Heats of solution and lattice-expansion and trapping energies of hydrogen in transition metals. Physical Review B, 1988, 38, 3690-3698.	1.1	96
98	Kiloâ€electronâ€volt Ar–ionâ€induced neutral atom desorption from Rh{331}: Relation of angular distributions to surface structure. Journal of Chemical Physics, 1988, 89, 2539-2543.	1.2	14
99	Corrections to the effective-medium theory of embedding energies: Interstitial hydrogen in metals. Physical Review B, 1988, 38, 1077-1086.	1.1	5
100	Interaction of H and D with the (001) surfaces of LiF and NaCl. Physical Review B, 1988, 38, 7759-7764.	1.1	10
101	Solubility of hydrogen in liquid aluminium. Materials Science and Technology, 1988, 4, 1-4.	0.8	43
102	Theory of Magnetic Excitations in Disordered Systems. Modern Problems in Condensed Matter Sciences, 1988, , 109-175.	0.1	5
103	Calculating Barriers to Oxygen Penetration on Metal Oxides with the Effective-Medium Theory. Materials Research Society Symposia Proceedings, 1988, 141, 279.	0.1	0
104	The Embedded Atom Method: Theory and Application. Materials Research Society Symposia Proceedings, 1988, 141, 31.	0.1	8
105	Beyond the Embedded Atom Interatomic Potential. Materials Research Society Symposia Proceedings, 1988, 141, 43.	0.1	1
106	The Interaction of an Atom with a Surface: A Model Based on Effective Medium Theory. Materials Research Society Symposia Proceedings, 1988, 141, 443.	0.1	0
107	The effective-medium theory beyond the nearest-neighbour interaction. Journal of Physics Condensed Matter, 1989, 1, 9765-9777.	0.7	27
108	Comparison of the interactions ofH2and rare-gas atoms with surfaces of insulators. Physical Review B, 1989, 39, 3854-3861.	1.1	19

#	Article	IF	CITATIONS
109	Theoretical study of hydrogen adsorption on Ru(0001): Possible surface and subsurface occupation sites. Physical Review B, 1989, 39, 5623-5631.	1.1	48
110	Application of molecular dynamics to the study of hydrogen embrittlement in Ni-Cr-Fe alloys. Physical Review B, 1989, 40, 10322-10336.	1.1	51
111	Theoretical calculations of He scattering intensities from MgO. Physical Review B, 1989, 39, 11131-11134.	1.1	1
112	Binding of charged particles in lattice defects. Physical Review B, 1989, 40, 11493-11495.	1.1	1
113	Crystal-melt and melt-vapor interfaces of nickel. Physical Review B, 1989, 40, 924-932.	1.1	75
114	A many-body embedded atom potential for describing ejection of atoms from surfaces. Radiation Effects and Defects in Solids, 1989, 109, 287-292.	0.4	3
115	The solubility of hydrogen in solid binary aluminum-lithium alloys. Metallurgical and Materials Transactions B - Process Metallurgy and Materials Processing Science, 1989, 20, 523-533.	0.5	19
116	Transport processes in solids during ion implantation. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1989, 115, 1-10.	2.6	11
117	Ion-beam studies of hydrogen-metal interactions. Journal of Nuclear Materials, 1989, 165, 9-64.	1.3	179
118	A theoretical study of the structure and reactivity of carbon and graphite layers on nickel surfaces. Surface Science Letters, 1989, 221, A502.	0.1	5
119	Determination of the full Heî—,Pt(110)(1 × 2) interaction potential from analyses of helium diffraction intensities. Surface Science Letters, 1989, 222, L837-L844.	0.1	0
120	The adsorption of H2, D2 and Ar on graphite: New theoretical results. Surface Science Letters, 1989, 208, L73-L79.	0.1	0
121	Heat of solution and site energies of hydrogen in disordered transition-metal alloys. Physical Review B, 1989, 40, 1481-1494.	1.1	33
122	The adsorption of H2, D2 and Ar on graphite: New theoretical results. Surface Science, 1989, 208, L73-L79.	0.8	13
123	Calculation of reaction rates and kinetic isotope effects for dissociative chemisorption of H2 and D2 on Ni(100), Ni(110), and Ni(111) surfaces. Surface Science, 1989, 214, 523-559.	0.8	41
124	Determination of the full He-Pt(110)($1\tilde{A}$ —2) interaction potential from analyses of helium diffraction intensities. Surface Science, 1989, 222, L837-L844.	0.8	24
125	Effective-medium theory of chemical binding: Delimitations on its use and application to hydrogen in GaAs and Si. Surface Science, 1989, 214, 1-16.	0.8	2
126	A theoretical study of the structure and reactivity of carbon and graphite layers on nickel surfaces. Surface Science, 1989, 221, 69-90.	0.8	25

ARTICLE IF CITATIONS # Multiple deuterium occupancy of vacancies in Pd and related metals. Physical Review B, 1989, 40, 127 1.1 92 1990-1992. Model of metallic cohesion: The embedded-atom method. Physical Review B, 1989, 39, 7441-7452. 1.1 Diffusion of hydrogen to a crack tip. Philosophical Magazine A: Physics of Condensed Matter, 129 0.8 9 Structure, Defects and Mechanical Properties, 1989, 59, 161-170. Theoretical Calculations on the Stability of Carbide Layers at Transition Metal Surfaces. Studies in Surface Science and Catalysis, 1989, 48, 335-345. Application of the Embedded Atom Method to Pb and Be. Materials Research Society Symposia 131 0.1 2 Proceedings, 1990, 193, 83. Structure and Dynamics of Aluminum Clusters. Materials Research Society Symposia Proceedings, 0.1 1990, 206, 209, Surface Melting and Surface Diffusion on Clusters. Materials Research Society Symposia Proceedings, 133 0.1 13 1990, 206, 241. Effect of Hydrogen on The Electronic Structure of a Grain Boundary In Iron. Materials Research 134 0.1 Society Symposia Proceedings, 1990, 209, 53. Interaction of hydrogen isotopes with metals: Deuterium trapped at lattice defects in palladium. 135 0.5 20 Journal of Fusion Energy, 1990, 9, 257-261. The dynamics of molecule-surface interaction. Computer Physics Reports, 1990, 12, 383-450. 2.3 Electrostatic field effects in surface reactivity: adsorption, dissociation and catalytic reaction of 137 0.1 3 nitric oxide. Surface Science Letters, 1990, 246, A166. Effective-medium calculations for hydrogen in Ni, Pd, and Pt. Physical Review B, 1990, 41, 12413-12423. 138 1.1 Surface melting of Ni(110). Physical Review B, 1990, 41, 439-450. 139 1.1 137 Strength of grain boundaries in impure metals. Materials Science and Technology, 1990, 6, 325-329. 140 0.8 The contribution made by surface science to understanding reactivity in heterogeneous catalysis. 141 17 1.7 Journal of the Chemical Society, Faraday Transactions, 1990, 86, 2675. Beyond Pair Potentials in Elemental Transition Metals and Semiconductors. Solid State Physics, 1990, 142 43, 1-91. Many-body anharmonic interactions in Ag and Ni. Philosophical Magazine A: Physics of Condensed 143 0.8 2 Matter, Structure, Defects and Mechanical Properties, 1990, 62, 377-385. Corrected effective medium calculations of the chemisorption of H and N on Fe(100), Fe(110) and 144 W(110). Surface Science, 1990, 235, 84-106.

#	Article	IF	CITATIONS
145	Indirect interactions of H/Ni(111) and H/Pd(100) using embedded atom method. Surface Science, 1990, 227, 114-122.	0.8	34
146	Resonant scattering of He-atoms from missing-row reconstructed Pt(110)1 × 2: comparison of theory and experiment. Surface Science, 1990, 236, L365-L368.	0.8	17
147	The bonding of hydrogen on nickel studied by inverse photoemission. Surface Science, 1990, 236, 250-258.	0.8	26
148	Interaction of H2 with simple metal surfaces: a model based on the anisotropic effective medium theory. Surface Science, 1990, 239, L505-L510.	0.8	6
149	The energetics and structure of nickel clusters: Size dependence. Journal of Chemical Physics, 1991, 94, 7376-7396.	1.2	359
150	The interaction potential and derived scattering and thermodynamic quantities of H2 with the MgO(001) surface. Surface Science, 1991, 247, 51-57.	0.8	3
151	Aspects of molecule-surface interactions. Surface Science, 1991, 242, 365-375.	0.8	6
152	Electrostatic field effects in surface reactivity: Adsorption, dissociation and catalytic reaction of nitric oxide. Surface Science, 1991, 246, 125-134.	0.8	30
153	Study of misfit dislocations at the interface of weakly bonded metal/metal systems. Acta Metallurgica Et Materialia, 1991, 39, 373-382.	1.9	22
154	Change in the work function of zirconium by oxidation at high temperatures and low oxygen pressures. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1399.	1.7	4
155	Environment Sensitive Embedding Energies of Impurities, and Grain Boundary Relaxation in Iron. Materials Research Society Symposia Proceedings, 1991, 238, 481.	0.1	1
156	Effect of hydrogen on the electronic structure of a grain boundary in iron. Solid State Communications, 1991, 79, 113-117.	0.9	37
157	Transition metal bonding functions and their application in adsorptions and catalytic reactions. Journal of Molecular Catalysis, 1991, 64, 53-84.	1.2	6
158	Empirical many-body interatomic potential for bcc transition metals. Physical Review B, 1991, 43, 6952-6961.	1.1	120
159	Interface effects of hydrogen uptake in Mo/V single-crystal superlattices. Physical Review B, 1991, 43, 6440-6445.	1.1	68
160	Analytic embedded-atom potentials for fcc metals: Application to liquid and solid copper. Physical Review B, 1991, 43, 4653-4658.	1.1	175
161	Charge transfer in transition-metal alloying: Charge-tailing effects. Physical Review B, 1991, 43, 1446-1454.	1.1	20
162	Hydrogen segregation and trapping in the Al/Si(111) interface. Physical Review B, 1991, 44, 1861-1874.	1.1	21

#	Article	IF	Citations
163	Surface premelting of Cu(110). Physical Review B, 1991, 44, 3226-3239.	1.1	106
164	Rare Gases on Graphite. Physics and Chemistry of Materials With Low-dimensional Structures, 1992, , 219-260.	1.0	6
165	Ab initiopotential for solids. Physical Review B, 1992, 46, 3798-3809.	1.1	43
166	Chapter 4 Surface States on Metals. Studies in Surface Science and Catalysis, 1992, , 99-143.	1.5	8
167	Surface melting of clusters and implications for bulk matter. Physical Review A, 1992, 45, 7969-7980.	1.0	182
168	Electronic structure of metallic superlattices: Mo/V. Physical Review B, 1992, 45, 1857-1868.	1.1	13
170	The quantum-chemical basis of the catalytic reactivity of transition metals. Philosophical Transactions of the Royal Society: Physical and Engineering Sciences, 1992, 341, 269-282.	1.0	11
171	First-principles study of He in Si. Physical Review B, 1992, 46, 12806-12809.	1.1	52
172	Comparison of the stability of small clusters of hydrogen near a Pd(001) or a Ni(001) surface. Surface Science, 1992, 269-270, 1116-1120.	0.8	6
173	Hydrogen interactions with defects in crystalline solids. Reviews of Modern Physics, 1992, 64, 559-617.	16.4	471
174	Energy effects and charge transfer in metal physics; modelling in real space. Physica B: Condensed Matter, 1992, 182, 1-17.	1.3	82
175	Deuterium permeation in polycrystalline nickel pre-implanted with nickel and helium ions. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1992, 158, 71-78.	2.6	0
176	Pseudo-molecular dynamics study of grain boundary segregation. Acta Mechanica Sinica/Lixue Xuebao, 1992, 8, 1-10.	1.5	0
177	The physics of simple metal clusters: self-consistent jellium model and semiclassical approaches. Reviews of Modern Physics, 1993, 65, 677-732.	16.4	1,557
178	Molecular dynamics of nanoscale layered structures. Scripta Materialia, 1993, 3, 479-498.	0.5	0
179	Molecular-dynamics study of the binding energy and melting of transition-metal clusters. Physical Review B, 1993, 48, 8253-8262.	1.1	132
180	The embedded-atom method: a review of theory and applications. Materials Science and Engineering Reports, 1993, 9, 251-310.	5.8	1,343
181	Constant-volume pair potential for Al–transition-metal compounds. Physical Review B, 1993, 47, 2961-2969.	1.1	14

	CHATION	REPORT	
#	Article	IF	Citations
182	Finite-temperature properties of sodium clusters. Physical Review B, 1993, 48, 2721-2732.	1.1	73
183	First-principles study of potassium adsorption on graphite. Physical Review B, 1993, 47, 13713-13721.	1.1	63
184	Anharmonic effects at the Ni(100) surface. Physical Review B, 1993, 47, 4127-4130.	1.1	14
185	Hydrogen Uptake in Mo/V Multi Layered Single-Crystal Superlattices — The Role of Charge Transfer at Interfaces*. Zeitschrift Fur Physikalische Chemie, 1993, 181, 343-351.	1.4	17
186	A molecular-dynamics simulation of crack-tip extension: The brittle-to-ductile transition. Modelling and Simulation in Materials Science and Engineering, 1994, 2, 865-892.	0.8	85
187	Low-angle neutron and x-ray scattering of hydrogenated and deuterated Mo/V superlattices. Physical Review B, 1994, 50, 11223-11226.	1.1	15
188	Theory of the location and associated hyperfine properties of the positive muon inLa2CuO4. Physical Review B, 1994, 49, 9879-9884.	1.1	30
189	Effective-medium tight-binding model for silicon. Physical Review B, 1994, 50, 10727-10741.	1.1	27
190	Surface anharmonicities and disordering on Ni(100) and Ni(110). Physical Review B, 1994, 50, 12084-12103.	1.1	21
191	Conduction-electron effect in quantum tunneling diffusion of hydrogen on metal surfaces. Physical Review B, 1994, 50, 11279-11282.	1.1	9
192	Electronic distortion in keV particle bombardment. Journal of Chemical Physics, 1994, 100, 8437-8443.	1.2	14
193	Evolution of the structural stability of large Cu, Ni, Pd, and Ag clusters with size: An analysis within the embedded atom method. Journal of Cluster Science, 1994, 5, 287-302.	1.7	21
194	Analytic embedded-atom potentials for bcc metals: application to calculating the thermodynamic data of bcc alloys. Physics Letters, Section A: General, Atomic and Solid State Physics, 1994, 192, 79-86.	0.9	17
195	Atomic-level computer simulation. Journal of Nuclear Materials, 1994, 216, 265-274.	1.3	16
196	Theory of location and associated hyperfine properties of the positive muon in La2CuO4. Hyperfine Interactions, 1994, 84, 87-103.	0.2	11
198	Effect of adsorption of EAM metal atoms on the structure of a sodium-alumino silicate glass surface: a molecular dynamics simulation. Surface Science, 1994, 319, 381-393.	0.8	14
199	Theory of adsorption and adsorbate-induced reconstruction. Surface Science, 1994, 299-300, 690-705.	0.8	38
200	Fourth moment approximation to tight binding: application to bcc transition metals. Surface Science, 1994, 301, 371-385.	0.8	39

#	Article	IF	CITATIONS
201	Theory of positrons in solids and on solid surfaces. Reviews of Modern Physics, 1994, 66, 841-897.	16.4	961
202	Embedded-atom method applied to bimetallic clusters: The Cu-Ni and Cu-Pd systems. Physical Review B, 1994, 49, 16649-16658.	1.1	50
203	Environment Sensitive Embedding Energies of Impurities, and Grain Boundary Stability in Tantalum. Materials Research Society Symposia Proceedings, 1995, 408, 291.	0.1	0
204	A Model B.C.C. Iron Including Angular Interactions. The Selfâ€Interstitial. Physica Status Solidi (B): Basic Research, 1995, 191, 249-266.	0.7	9
205	A multisite interaction expansion of the total energy in metals. Nuclear Instruments & Methods in Physics Research B, 1995, 102, 1-2.	0.6	3
206	Charge transfer at interfaces inMoxV1â^'x/V superlattices. Physical Review B, 1995, 52, 10792-10795.	1.1	13
207	Concepts in Theoretical Heterogeneous Catalytic Reactivity. Catalysis Reviews - Science and Engineering, 1995, 37, 557-698.	5.7	278
208	Interactions Between Adsorbate Particles. Handbook of Surface Science, 1996, , 577-650.	0.3	21
209	Clobal potentials for calcium and strontium solids. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 425.	1.7	24
210	Theory of chemisorption and reactions on metal surfaces. Surface Science Reports, 1996, 24, 55-124.	3.8	296
211	Dynamics of H2 dissociation on Cu(100): Effects of surface defects. Journal of Chemical Physics, 1996, 104, 9994-10000.	1.2	12
212	ELECTRON THEORY OF METALS. , 1996, , 47-133.		7
213	The orientation dependence of the hydrogen distribution within Mo/V (110) and (001) multilayered artificial superlattices. Journal of Physics Condensed Matter, 1997, 9, 73-85.	0.7	7
214	Hydrogen-induced lattice expansion of vanadium in a Fe/V (001) single-crystal superlattice. Physical Review B, 1997, 55, 15905-15911.	1.1	49
215	A molecular orbital study of H interaction with an edge dislocation in Fe bcc. Modelling and Simulation in Materials Science and Engineering, 1997, 5, 357-363.	0.8	13
216	The Low Temperature Adsorption of Oxygen on Rh(111). Zeitschrift Fur Physikalische Chemie, 1997, 198, 1-17.	1.4	20
219	On the cohesive approach to the calculation of d-metal on d-metal adsorption properties. Surface Science, 1997, 371, 157-167.	0.8	9
220	Vacancy formation in nickel and α-nickel-carbon alloy. Acta Materialia, 1997, 45, 4759-4764.	3.8	34

#	Article	IF	CITATIONS
221	Neutron spectroscopy study of the local modes of interstitials in transition metals. Physics of the Solid State, 1997, 39, 19-22.	0.2	1
222	The local orientational orders and structures of liquid and amorphous metals Au and Ni during rapid solidification. Physica B: Condensed Matter, 1997, 239, 267-273.	1.3	24
223	Local modes of interstitial atoms in transition metals. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1997, 230, 63-67.	2.6	6
224	Electric field effects in heterogeneous catalysis. Journal of Molecular Catalysis A, 1997, 119, 263-273.	4.8	57
225	Characterization of the electronic density of metals in terms of the bulk modulus. Journal of Materials Science, 1998, 33, 167-171.	1.7	14
226	Ab initiomolecular-dynamics studies of doped magic clusters and their interaction with atoms. Physical Review B, 1998, 57, 4939-4942.	1.1	59
227	Electronic structure and energetics of LaNi5, α-La2Ni10H and β-La2Ni10H14. Journal of Alloys and Compounds, 1998, 281, 81-91.	2.8	90
228	Reaction of oxygen and sulphur dioxide with Cu(100)-c(2×2)-Mn surface alloy. Surface Science, 1998, 408, 326-334.	0.8	29
229	A theory of hydrogen trapping in a faulted zone of FCC iron. Journal Physics D: Applied Physics, 1998, 31, 893-899.	1.3	14
230	Calculation of Mechanical, Thermodynamic and Transport Properties of Metallic Glass Formers. Materials Research Society Symposia Proceedings, 1998, 554, 43.	0.1	117
231	Energy Properties of Single Helium Atom in Metals by Effective-Medium Theory. Chinese Physics Letters, 1998, 15, 713-714.	1.3	1
232	Interaction between atoms and surfaces: A bond-pair description based on an extended Anderson model. Physical Review B, 1998, 58, 5007-5021.	1.1	36
233	Electronic Structure and Energetics of LaNi5, α-La2Ni10H and β-La2Ni10H14. Materials Research Society Symposia Proceedings, 1998, 513, 73.	0.1	0
234	Effects of varying compressive biaxial strain on the hydrogen uptake of thin vanadium (001) layers. Journal of Physics Condensed Matter, 1999, 11, 6669-6677.	0.7	13
235	Self-consistent screening of diatomic molecules in an electron gas. Physical Review B, 1999, 60, 2074-2083.	1.1	19
236	Thermal and mechanical properties of some fcc transition metals. Physical Review B, 1999, 59, 3468-3473.	1.1	129
237	The adiabatic molecule–metal surface interaction: Theoretical approaches. Reviews of Modern Physics, 1999, 71, 231-265.	16.4	133
238	Computational Materials Chemistry at the Nanoscale. Journal of Nanoparticle Research, 1999, 1, 51-69.	0.8	23

ARTICLE IF CITATIONS # Electronic structure and activation energy of hydrogen in NEG alloy using nonlinear response theory. Pramana - Journal of Physics, 1999, 52, 333-340. 239 0.9 0 Alloy surfaces: segregation, reconstruction and phase transitions. Computational Materials Science, 240 1.4 118 1999, 15, 196-235. Thermodynamic properties of hydrogen in Mo/V (110) superlattices: the dependence on 241 2.8 4 crystallographic orientation. Journal of Alloys and Compounds, 1999, 285, 21-26. Hydrogen on the Fe(110) surface and near bulk bcc Fe vacancies. Surface Science, 1999, 421, 1-16. 0.8 Calculation of diffusion barriers for helium atom in metals. Acta Physica Sinica (overseas Edition), 243 0.1 0 1999, 8, 746-753. Double Lattice Inversion Technique ? Application to the EAM Potential Construction. Physica Status Solidi (B): Basic Research, 2000, 222, 457-469. Environmental dependence of screened tight-binding parameters in La2Ni10H14. Journal of Alloys and 245 2.8 12 Compounds, 2000, 306, 113-121. Modified embedded atom method calculations for reconstructed (110) surfaces of face-centered cubic 246 0.8 21 metals. Surface Science, 2000, 445, 18-22. The electronic structure and bonding of hydrogen near a fcc Fe stacking fault. Journal Physics D: 247 1.3 9 Applied Physics, 2000, 33, 292-298. Embedded-atom-method functions for the body-centered-cubic iron and hydrogen. Journal of 248 1.2 58 Materials Research, 2001, 16, 3496-3502. A comparative study of the electronic structure of H pairs near a/2 and a[0 1 0] dislocations in bcc Fe. 249 7 3.1Applied Surface Science, 2001, 182, 103-114. Development of modified embedded atom potentials for the Cu–Ag system. Superlattices and 1.4 Microstructures, 2001, 30, 261-271. Plasma-material interactions in current tokamaks and their implications for next step fusion 251 1.6 1,185 reactors. Nuclear Fusion, 2001, 41, 1967-2137. Ab initio simulation of physisorption: N2 on pregraphitic clusters. Computational and Theoretical 1.5 Chemistry, 2001, 544, 221-235. Phase transitions of hydrogen in quasi-two-dimensional vanadium lattices. Journal of Physics 253 0.7 13 Condensed Matter, 2001, 13, 1685-1698. First-principles calculations of C14-type Laves phase Ti-Mn hydrides. Physical Review B, 2002, 66, . 254 1.1 34 H-H interactions in Nb/W(110) superlattices. Physical Review B, 2002, 66, . 255 1.1 9 First-principles study on3dtransition-metal dihydrides. Physical Review B, 2002, 65, . 1.1

#	Article	IF	CITATIONS
257	Oxygen-inducedp(2×3)reconstruction on Mo(112) studied by LEED and STM. Physical Review B, 2002, 65, .	1.1	53
258	Ab Initio Computer Simulations on Microclusters: Structures and Electronic Properties. Springer Series in Cluster Physics, 2002, , 9-88.	0.3	16
259	A new form of the Sutton–Chen potential for the Cu–Ag alloys. Superlattices and Microstructures, 2002, 31, 297-313.	1.4	6
260	Towards Multiscale Modeling of Metals via Embedded Particle Computer Simulation. Multiscale Modeling and Simulation, 2003, 1, 25-39.	0.6	8
261	Atomistic simulations of effect of hydrogen on kink-pair energetics of screw dislocations in bcc iron. Acta Materialia, 2003, 51, 1767-1773.	3.8	77
262	Molecular dynamics simulation on edge dislocation in the bulk and nanoparticles of iron. Computational Materials Science, 2003, 27, 333-341.	1.4	6
263	Influence of biaxial strain on thermodynamical properties of hydrogen in (001) oriented Mo/V superlattices. Journal of Alloys and Compounds, 2003, 356-357, 545-548.	2.8	5
264	Stability and clusterization of hydrogen-vacancy complexes inαâ~'Fe:Anab initiostudy. Physical Review B, 2003, 67, .	1.1	296
265	Atomic, Electron and Phonon Aspects of the Edge Dislocation in Iron. Defect and Diffusion Forum, 2004, 224-225, 37-44.	0.4	1
267	Analysis of the bonding and reactivity of H and the Al13 cluster using density functional concepts. Journal of Chemical Physics, 2003, 119, 5128-5141.	1.2	55
268	Thermophysical properties of liquid refractory metals: Comparison between hard sphere model calculation and electrostatic levitation measurements. Journal of Chemical Physics, 2003, 118, 7912-7920.	1.2	59
269	Molecular dynamics simulation of thermophysical properties of undercooled liquid cobalt. Journal of Physics Condensed Matter, 2004, 16, 2565-2574.	0.7	23
270	Hydrogen-induced defects in bulk niobium. Physical Review B, 2004, 69, .	1.1	77
271	Magnetooptic properties of Feâ^•Pd and Coâ^•Pd bilayers under hydrogen absorption. Applied Physics Letters, 2004, 85, 615-617.	1.5	23
272	Density of states induced by a hydrogenic impurity in a metal. International Journal of Hydrogen Energy, 2004, 29, 497-500.	3.8	2
273	The influence of electronic structure on hydrogen absorption in palladium alloys. Journal of Physics Condensed Matter, 2004, 16, 6267-6277.	0.7	75
274	Investigation of the formation of iron nanoparticles from the gas phase by molecular dynamics simulation. Nanotechnology, 2004, 15, 525-533.	1.3	98
275	Diffusion of interstitial hydrogen into and through bcc Fe from first principles. Physical Review B, 2004, 70, .	1.1	406

#	Article	IF	CITATIONS
276	Binding Energy and the Heat of Chemisorption on Metallic Catalysts — A Thermodynamic Aspect. Adsorption Science and Technology, 2005, 23, 161-172.	1.5	1
277	Hydrogen-Promoted Grain Boundary Embrittlement and Vacancy Activity in Metals: Insights from <i>Ab Initio</i> Total Energy Calculatons. Materials Transactions, 2005, 46, 756-760.	0.4	39
278	Interatomic Potentials for Metals. , 2005, , 459-478.		18
279	Phonon dispersions and elastic constants of disordered Pd–Ni alloys. Physica B: Condensed Matter, 2005, 355, 382-391.	1.3	9
280	Atomistic Computer Simulation of Diffusion. , 2005, , 113-171.		9
281	Thermodynamical and mechanical properties of Pd–Ag alloys. Computational Materials Science, 2005, 32, 107-117.	1.4	50
282	Atomistic Computer Simulation of Diffusion. , 2005, , 113-171.		1
283	Electronic Structure. Springer Series in Materials Science, 2005, , 401-437.	0.4	0
285	Molecular dynamics simulation of size and strain rate dependent mechanical response of FCC metallic nanowires. Nanotechnology, 2006, 17, 3451-3467.	1.3	162
286	Location and energy of interstitial hydrogen in the1â^•1approximantW-TiZrNiof the icosahedralTiZrNiquasicrystal: Rietveld refinement of x-ray and neutron diffraction data and density-functional calculations. Physical Review B, 2006, 73, .	1.1	7
287	3.4.1 Adsorbate properties of hydrogen on solid surfaces. , 0, , 1-130.		0
288	Nitrogen Absorption by Sm2Fe17. Journal of the Ceramic Society of Japan, 2006, 114, 896-901.	1.3	2
289	Embedded atom method potentials employing a faithful density representation. Modelling and Simulation in Materials Science and Engineering, 2006, 14, 721-731.	0.8	9
290	Homogeneous nucleation and growth from highly supersaturated vapor by molecular dynamics simulation. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2007, , 351-377.	0.1	0
291	Thin Films of Cross-Linked Metallo-Supramolecular Coordination Polyelectrolytes. Langmuir, 2007, 23, 12179-12184.	1.6	32
292	Transport Properties of Undercooled Liquid Copper: A Molecular Dynamics Study. International Journal of Thermophysics, 2008, 29, 1408-1421.	1.0	24
293	Hydrogen in <mml:math <br="" xmlns:mml="http://www.w3.org/1998/Math/MathML">display="inline"><mml:mi>α</mml:mi></mml:math> -iron: Stress and diffusion. Physical Review B, 2008, 78, .	1.1	67
294	Chapter 6 Structure of Isolated Clusters. Handbook of Metal Physics, 2008, 5, 143-173.	0.0	1

#	Article	IF	Citations
297	Hydrogen-vacancy complexes in electron-irradiated niobium. Physical Review B, 2009, 79, .	1.1	25
298	Low-temperature gas from marine shales. Geochemical Transactions, 2009, 10, 3.	1.8	9
299	Molecular dynamic studies on materials under laser shocks. Phase Transitions, 2009, 82, 167-190.	0.6	2
300	Melting Behaviour of Shell-symmetric Aluminum Nanoparticles: Molecular Dynamics Simulation. Chinese Journal of Chemical Physics, 2009, 22, 215-222.	0.6	2
301	Composition-dependent interatomic potentials: A systematic approach to modelling multicomponent alloys. Philosophical Magazine, 2009, 89, 3371-3391.	0.7	11
302	Structure of Adsorbents, Ion Exchangers, Ion Conductors, Catalysts, and Permeable Materials. , 2009, , 63-102.		0
303	Using Embedded-Atom Method (EAM) to Simulate Interaction of Intense Laser with Lead in LIBS. , 2010, , .		0
304	Atomistic properties of helium in hcp titanium: A first-principles study. Journal of Nuclear Materials, 2010, 402, 55-59.	1.3	18
305	First-principles study on dissolution and diffusion properties of hydrogen in molybdenum. Journal of Nuclear Materials, 2010, 404, 109-115.	1.3	49
306	First-principles energetics of hydrogen traps in α-Fe: Point defects. Acta Materialia, 2010, 58, 4730-4741.	3.8	174
307	H2 reactivity on the surfaces of In and Sn at 298K. Applied Surface Science, 2010, 256, 3321-3324.	3.1	0
308	Natural catalytic activity in a marine shale for generating natural gas. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2010, 466, 3527-3537.	1.0	7
309	Communications: Exceptions to the d-band model of chemisorption on metal surfaces: The dominant role of repulsion between adsorbate states and metal d-states. Journal of Chemical Physics, 2010, 132, 221101.	1.2	201
310	Force-matched embedded-atom method potential for niobium. Physical Review B, 2010, 81, .	1.1	120
311	First-principles calculations and tight-binding molecular dynamics simulations of the palladium-hydrogen system. Physical Review B, 2010, 81, .	1.1	8
312	<i>Ab initio</i> molecular dynamics simulation of hydrogen diffusion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>î±</mml:mi>-iron. Physical Review B, 2010, 81, .</mml:math 	1.1	46
313	Finite-temperature elasticity of fcc Al: Atomistic simulations and ultrasonic measurements. Physical Review B, 2011, 84, .	1.1	37
314	The size dependence of the mechanical properties and breaking behavior of metallic nanowires: A statistical description. Computational Materials Science, 2011, 50, 1418-1424.	1.4	20

#	Article	IF	CITATIONS
315	Hydrogen hardening effect in heavily deformed single crystal α-Fe. Computational Materials Science, 2011, 50, 3397-3402.	1.4	21
316	Hydrogenation properties of Ti–V–Mn alloys with a BCC structure containing high and low oxygen concentrations. Journal of Alloys and Compounds, 2011, 509, 1841-1847.	2.8	29
317	Concepts for simulating and understanding materials at the atomic scale. MRS Bulletin, 2012, 37, 477-484.	1.7	10
318	Interaction between impurity nitrogen and tungsten: a first-principles investigation. Chinese Physics B, 2012, 21, 016105.	0.7	18
319	Contributions of the embedded-atom method to materials science and engineering. MRS Bulletin, 2012, 37, 485-491.	1.7	24
320	Solute–point defect interactions in bcc systems: Focus on first principles modelling in W and RPV steels. Current Opinion in Solid State and Materials Science, 2012, 16, 115-125.	5.6	86
321	Multiple hydrogen trapping at monovacancies. Philosophical Magazine Letters, 2012, 92, 217-225.	0.5	22
322	Molecular Simulation of Dissociation Phenomena of Gas Molecule on Metal Surface. , 2012, , .		0
323	Single walled carbon nanotube growth and chirality dependence on catalyst composition. Nanoscale, 2013, 5, 9848.	2.8	22
324	Hydrogen absorption induced reversible effect on magneto-optical property of Pd/Fe, Pd/Co and Pd/Ni bilayers. Thin Solid Films, 2013, 531, 487-490.	0.8	17
325	Behaviors of helium in vanadium: Stability, diffusion, vacancy trapping and ideal tensile strength. Progress in Natural Science: Materials International, 2013, 23, 459-463.	1.8	14
326	Current understanding of the growth of carbon nanotubes in catalytic chemical vapour deposition. Carbon, 2013, 58, 2-39.	5.4	460
327	Investigation of Catalytic Finite-Size-Effects of Platinum Metal Clusters. Journal of Physical Chemistry Letters, 2013, 4, 222-226.	2.1	249
328	Trapping and diffusion behaviors of helium at vacancy in iron from first principles. Science China: Physics, Mechanics and Astronomy, 2013, 56, 1100-1106.	2.0	7
329	Site-Specific Scaling Relations for Hydrocarbon Adsorption on Hexagonal Transition Metal Surfaces. Journal of Physical Chemistry C, 2013, 117, 20078-20088.	1.5	36
330	First-principles study of temperature-dependent diffusion coefficients for helium in α-Ti. Journal of Applied Physics, 2013, 114, 153507.	1.1	11
331	Nano-Voids Formation and Hydrogen Configuration in Low Frictional Cr-Mo Layers Electrodeposited with Organic Sulfonic Acid Catalyst. Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals, 2013, 77, 527-536.	0.2	2
332	Grain boundary migration of substitutional and interstitial atoms in α-iron. Acta Materialia, 2014, 69, 105-113.	3.8	39

#	Article	IF	CITATIONS
333	Gupta potential for alkaline earth metals: Calcium and strontium. Computational Materials Science, 2014, 85, 142-146.	1.4	4
334	Hierarchy of Chemical Bonding in the Synthesis of Fe-Phthalocyanine on Metal Surfaces: A Local Spectroscopy Approach. Journal of Physical Chemistry Letters, 2014, 5, 3175-3182.	2.1	36
335	Peridynamic State-Based Models and the Embedded-Atom Model. Communications in Computational Physics, 2014, 15, 179-205.	0.7	23
336	An accurate full-dimensional potential energy surface for H–Au(111): Importance of nonadiabatic electronic excitation in energy transfer and adsorption. Journal of Chemical Physics, 2015, 143, 124708.	1.2	62
337	Fundamental aspects of deuterium retention in tungsten at high flux plasma exposure. Journal of Applied Physics, 2015, 118, .	1.1	55
338	Energetics and heterodiffusion of Cu on Ag(110) stepped surfaces. Surface and Interface Analysis, 2015, 47, 855-862.	0.8	11
339	Systematic analysis and modification of embedded-atom potentials: case study of copper. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 074001.	0.8	7
340	First-principles investigation of hydrogen trapping and diffusion at grain boundaries in nickel. Acta Materialia, 2015, 98, 306-312.	3.8	132
341	The dislocation core misfit potential. Computational Materials Science, 2015, 100, 195-202.	1.4	1
342	Large-Scale Computations in Chemistry: A Bird's Eye View of a Vibrant Field. Chemical Reviews, 2015, 115, 5797-5890.	23.0	182
343	The temperature-dependent diffusion coefficient of helium in zirconium carbide studied with first-principles calculations. Journal of Applied Physics, 2015, 117, .	1.1	13
344	Hydrogen permeance studies in ordered ternary Cu–Pd alloys. International Journal of Hydrogen Energy, 2015, 40, 14885-14899.	3.8	11
345	Optimum temperature on structural growth of multiwalled carbon nanotubes with low activation energy. Diamond and Related Materials, 2015, 58, 129-138.	1.8	20
346	A Gupta potential for magnesium in hcp phase. Computational Materials Science, 2015, 98, 328-332.	1.4	11
347	Statistical model and first-principles simulation on concentration of He V cluster and He bubble formation in α-Fe and W. Journal of Nuclear Materials, 2015, 456, 162-173.	1.3	20
348	Analyzing relationships between surface perturbations and local chemical reactivity of metal sites: Alkali promotion of O2 dissociation on Ag(111). Journal of Chemical Physics, 2016, 144, 234704.	1.2	13
349	Theoretical Heterogeneous Catalysis: Scaling Relationships and Computational Catalyst Design. Annual Review of Chemical and Biomolecular Engineering, 2016, 7, 605-635.	3.3	303
350	Effect of CVD Process Temperature on Activation Energy and Structural Growth of MWCNTs. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2016, 47, 1413-1424	1.1	5

#	Article	IF	CITATIONS
351	Annealing-induced alloy formation in Pd/Fe bilayers on Si(1 1 1) for hydrogen sensing. Applied Surface Science, 2016, 366, 38-45.	3.1	6
352	On-Surface Synthesis of Phthalocyanine Compounds. Advances in Atom and Single Molecule Machines, 2016, , 115-129.	0.0	1
353	Ab initio study of He-He interactions in homogeneous electron gas. Nuclear Instruments & Methods in Physics Research B, 2017, 393, 140-143.	0.6	2
354	Genetic algorithm approach to global optimization of the full-dimensional potential energy surface for hydrogen atom at fcc-metal surfaces. Chemical Physics Letters, 2017, 683, 286-290.	1.2	19
355	Mechanisms of hydrogen embrittlement in steels: discussion. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20170032.	1.6	21
356	Relationship between element-selective electronic states and hydrogen absorption properties of Pd-M(M=Ru,Rh,Ag,and Au)alloys. Physical Review B, 2017, 95, .	1.1	9
357	Identifying "Optimal―Electrocatalysts: Impact of Operating Potential and Charge Transfer Model. ACS Catalysis, 2017, 7, 8641-8652.	5.5	21
358	Hydrogenation effect on uniaxial magnetic anisotropy of a Co Pd1â~' alloy microstructure. Journal of Alloys and Compounds, 2017, 695, 2365-2373.	2.8	18
359	Hydrogen trapping in MAX phase Ti ₃ SiC ₂ : Insight from chemical bonding by density functional theory. Europhysics Letters, 2017, 118, 47002.	0.7	2
360	Molecular-dynamics simulations of binary Pd-Si metal alloys: Glass formation, crystallisation and cluster properties. Journal of Non-Crystalline Solids, 2018, 487, 72-86.	1.5	21
361	Characterization of lattice defects in metallic materials by positron annihilation spectroscopy: A review. Journal of Materials Science and Technology, 2018, 34, 577-598.	5.6	127
362	Behaviors of helium in Cr ₂ AlC from first principles. Journal of the American Ceramic Society, 2018, 101, 5771-5780.	1.9	10
363	Simulation on the Factors Affecting the Crystallization Process of FeNi Alloy by Molecular Dynamics. ACS Omega, 2019, 4, 14605-14612.	1.6	23
364	Ferromagnetic ligand holes in cobalt perovskite electrocatalysts as an essential factor for high activity towards oxygen evolution. Physical Chemistry Chemical Physics, 2019, 21, 2977-2983.	1.3	32
365	Factors affecting the structure, phase transition and crystallization process of AlNi nanoparticles. Journal of Alloys and Compounds, 2020, 812, 152133.	2.8	25
366	Origin of Electronic Modification of Platinum in a Pt ₃ V Alloy and Its Consequences for Propane Dehydrogenation Catalysis. ACS Applied Energy Materials, 2020, 3, 1410-1422.	2.5	41
367	Data-driven acceleration of first-principles saddle point and local minimum search based on scalable Gaussian processes. , 2020, , 119-168.		0
368	Beyond the static corrugation model: Dynamic surfaces with the embedded atom method. Journal of Chemical Physics, 2021, 154, 074710.	1.2	7

		CITATION REPORT		
#	Article		IF	CITATIONS
369	Effectively one-dimensional phase diagram of CuZr liquids and glasses. Physical Review	B, 2021, 103, .	1.1	4
370	Infusing theory into deep learning for interpretable reactivity prediction. Nature Comm 2021, 12, 5288.	unications,	5.8	38
371	Classical and First Principles Molecular Dynamics Simulations in Material Science: Appli Structural and Dynamical Properties of Free and Supported Clusters. NATO ASI Series S 1996, , 295-324.	cation to Feries B: Physics,	0.2	1
372	Atomistic Simulations of Surfaces and Interfaces. , 1992, , 89-122.			4
373	Embedded Atom Method: Many-Atom Description of Metallic Cohesion. , 1989, , 181-1	91.		10
374	Theory of Adsorption-Desorption Kinetics and Dynamics. , 1990, , 567-598.			1
375	Theoretical Aspects of Adsorption. , 1990, , 213-254.			2
376	Electronic Theory of Chemisorption. , 1990, , 255-323.			4
377	Implantation, Retention and Release of Hydrogen Isotopes in Solids. , 1986, , 439-494.			12
378	Structural and Dynamical Aspects of Adsorption and Desorption. Topics in Current Phys 301-346.	sics, 1987, ,	0.5	4
379	Adsorption Phenomena. , 1996, , 411-538.			3
380	The Embedded Atom Method: A Review. Springer Proceedings in Physics, 1990, , 48-63		0.1	5
381	The Binding of Adsorbates to Metal Surfaces. Springer Series in Surface Sciences, 1985	,,18-28.	0.3	3
382	Electronic Structure. Springer Series in Materials Science, 1993, , 300-320.		0.4	1
383	Surface Science Model Studies of the Electrochemical Interface. , 1986, , 255-280.			7
384	How We and Molecules Explore Molecular Landscapes. Jerusalem Symposia on Quantu Biochemistry, 1991, , 1-15.	m Chemistry and	0.2	2
385	Quantum Mechanical Calculations of Chemical Interactions on Transition Metal Surface 253-359.	25. , 1992, ,		3
386	CHEMISORPTION AND REACTIVITY OF METALS. , 1984, , 93-144.			4

# 387	ARTICLE Cluster Simulations: Melting and Sintering. , 1993, , 227-241.	IF	CITATIONS
388	Testing an interatomic force model. , 2003, , 129-157.		1
389	Hybrid Schemes. , 2003, , 253-262.		1
390	Solubility of hydrogen in liquid aluminium. Materials Science and Technology, 1988, 4, 1-4.	0.8	11
391	Strength of grain boundaries in impure metals. Materials Science and Technology, 1990, 6, 325-329.	0.8	2
392	Hydrogen Interaction with Vacancies in Electron Irradiated Niobium. Acta Physica Polonica A, 2008, 113, 1293-1299.	0.2	5
393	Grain-Boundary Diffusion of Hydrogen Atoms in the \$alpha\$-Iron. Metallofizika I Noveishie Tekhnologii, 2016, 36, 1399-1410.	0.2	6
394	Hydrogen in amorphous Ni–Zr: Pressure concentration isotherms, site occupation, and binding energies. Journal of Materials Research, 1986, 1, 765-773.	1.2	37
395	Ionic Models. , 2003, , 263-274.		0
396	Essential Quantum Mechanics. , 2003, , 3-63.		0
397	Pairwise potentials in simple metals. , 2003, , 158-186.		0
398	Essential Density Functional Theory. , 2003, , 64-78.		0
399	Linear Response Theory. , 2003, , 96-126.		1
400	Tight Binding. , 2003, , 187-252.		0
401	Exploiting the Variational Principle. , 2003, , 79-95.		1
402	è;¨é¢åŒ–å¦åå;œã«ãŠãťā,‹ä»•ä⁰‹é–¢æ•°ã®å½¹å‰². Shinku/Journal of the Vacuum Society of Japan, 2005, 48, 54	₽0 £1 8.	0
404	Using EAM to simulate interaction of intense laser LIBS in lead. , 2010, , .		0
405	Interatomic Potentials, Scattering and Nuclear Stopping. Springer Series in Solid-state Sciences, 2014, , 235-280.	0.3	0

	CITATION	REPORT	
#	Article	IF	CITATIONS
406	Some Applications of the Density-Functional Formalism to Chemisorption. , 1984, , 515-530.		0
407	CALCULATION OF SMALL ENERGY CHANGES FOR ADSORBATES AT SURFACES. , 1984, , 145-158.		0
408	Density Functionals and the Description of Metal Surfaces. , 1985, , 233-263.		0
409	The Interaction of Aromatic Molecules with the Basal Plane of Graphite and Rare Gas Atoms. Springer Series in Surface Sciences, 1989, , 122-127.	0.3	0
411	Application of the Tight-Binding Bond Model. , 1989, , 369-380.		0
412	The Effective-Medium Theory. Springer Proceedings in Physics, 1990, , 34-47.	0.1	Ο
413	Effective-Medium Theory: Considering Corrections and Delimitations. Springer Proceedings in Physics, 1990, , 232-241.	0.1	0
414	Adsorption Phenomena. Springer Series in Surface Sciences, 1993, , 381-498.	0.3	0
415	Quantum Molecular Dynamics Studies of the Structure and Dynamics of Metal Clusters. , 1993, , 127-142.		0
416	Molecular Dynamics of Nanophase Intermetallics. , 1994, , 315-322.		0
417	Production of Nitrides and Carbides by Gas-Phase Interstitial Modification. , 1995, , 371-409.		1
418	Solid Solution. , 2016, , 1-9.		2
419	Molecular Dynamics Study of the Hydrogen and Carbon Effect on Mobility of Grain Boundaries in \$alpha\$-Iron. Metallofizika I Noveishie Tekhnologii, 2019, 41, 1187-1203.	0.2	0
420	Molecular Vibrations at Surfaces. Springer Series in Chemical Physics, 1983, , 14-23.	0.2	Ο
422	Iron oxide-Palladium core-shell nanospheres for ferromagnetic resonance-based hydrogen gas sensing. International Journal of Hydrogen Energy, 2022, 47, 8155-8163.	3.8	4
423	Effective medium theory for bcc metals: electronically non-adiabatic H atom scattering in full dimensions. Physical Chemistry Chemical Physics, 2022, 24, 8738-8748.	1.3	5
424	A Career in Catalysis: Jens Kehlet NÃ,rskov. ACS Catalysis, 2022, 12, 9679-9689.	5.5	19
428	Interatomic potentials: achievements and challenges. Advances in Physics: X, 2023, 8, .	1.5	11

#	Article	IF	CITATIONS
429	Carbon Nanotube Growth Mechanisms. , 2022, , 57-87.		0
431	Extremely Shallow Valence Band in Lanthanum Trihydride. Journal of the American Chemical Society, 2023, 145, 560-566.	6.6	0
432	(n, m) Distribution of Single-Walled Carbon Nanotubes Grown from a Non-Magnetic Palladium Catalyst. Molecules, 2023, 28, 2453.	1.7	1
433	Solid Solution. , 2023, , 1-9.		0