

Michael Weinert

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227
papers

11,660
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53
h-index

102
g-index

230
ext. papers

12,267
ext. citations

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L-index

#	Paper	IF	Citations
227	Full-potential self-consistent linearized-augmented-plane-wave method for calculating the electronic structure of molecules and surfaces: O ₂ molecule. <i>Physical Review B</i> , 1981 , 24, 864-875	3.3	1836
226	Total-energy all-electron density functional method for bulk solids and surfaces. <i>Physical Review B</i> , 1982 , 26, 4571-4578	3.3	861
225	Surface magnetism of Fe(001). <i>Physical Review B</i> , 1983 , 28, 6741-6748	3.3	376
224	Prediction of Electronic Interlayer States in Graphite and Reinterpretation of Alkali Bands in Graphite Intercalation Compounds. <i>Physical Review Letters</i> , 1983 , 50, 761-764	7.4	302
223	Solution of Poisson's equation: Beyond Ewald-type methods. <i>Journal of Mathematical Physics</i> , 1981 , 22, 2433-2439	1.2	267
222	Fractional occupations and density-functional energies and forces. <i>Physical Review B</i> , 1992 , 45, 13709-13712	3.3	253
221	Surface barrier for electrons in metals. <i>Physical Review B</i> , 1988 , 37, 6113-6120	3.3	240
220	Tunneling spectroscopy of bcc (001) surface states. <i>Physical Review Letters</i> , 1995 , 75, 2960-2963	7.4	237
219	Total-energy differences and eigenvalue sums. <i>Physical Review B</i> , 1985 , 32, 2115-2119	3.3	216
218	Ferromagnetism and antiferromagnetism of 3d-metal overlayers on metals. <i>Physical Review Letters</i> , 1988 , 60, 1077-1080	7.4	207
217	Distance of the image plane from metal surfaces. <i>Physical Review B</i> , 1989 , 40, 7565-7573	3.3	180
216	Tuning Dirac states by strain in the topological insulator Bi ₂ Se ₃ . <i>Nature Physics</i> , 2014 , 10, 294-299	16.2	174
215	Interface magnetism in metals: Ag/Fe(001). <i>Physical Review B</i> , 1984 , 30, 36-43	3.3	173
214	Hybridization-induced band gaps in transition-metal aluminides. <i>Physical Review B</i> , 1998 , 58, 9732-9740	3.3	161
213	Local stability of nonequilibrium phases. <i>Physical Review Letters</i> , 1994 , 72, 3076-3079	7.4	153
212	Role of an interfacial FeO layer in the electric-field-driven switching of magnetocrystalline anisotropy at the Fe/MgO interface. <i>Physical Review B</i> , 2010 , 81,	3.3	151
211	Fast and selective room-temperature ammonia sensors using silver nanocrystal-functionalized carbon nanotubes. <i>ACS Applied Materials & Interfaces</i> , 2012 , 4, 4898-904	9.5	144

210	Core-level shifts in bulk alloys and surface adlayers. <i>Physical Review B</i> , 1995 , 51, 17168-17180	3.3	135
209	Frozen-phonon total-energy determination of structural surface phase transitions: W(001). <i>Physical Review Letters</i> , 1985 , 54, 2261-2264	7.4	132
208	Linearized augmented-plane-wave calculation of the electronic structure and total energy of tungsten. <i>Physical Review B</i> , 1985 , 32, 7792-7797	3.3	132
207	Epitaxial graphene on SiC(0001): more than just honeycombs. <i>Physical Review Letters</i> , 2010 , 105, 085502	7.4	117
206	Indium-doped SnO ₂ nanoparticle-graphene nanohybrids: simple one-pot synthesis and their selective detection of NO ₂ . <i>Journal of Materials Chemistry A</i> , 2013 , 1, 4462	13	113
205	First-principles calculation of impurity-solution energies in Cu and Ni. <i>Physical Review B</i> , 1989 , 39, 930-933	3.3	109
204	Transition-metal aluminide formation: Ti, V, Fe, and Ni aluminides. <i>Physical Review B</i> , 1998 , 58, 5981-5988	3.3	106
203	Vacancies and impurities in aluminum and magnesium. <i>Physical Review B</i> , 1995 , 52, 6313-6326	3.3	106
202	Cesiation of W(001): Work Function Lowering by Multiple Dipole Formation. <i>Physical Review Letters</i> , 1982 , 48, 1128-1131	7.4	99
201	Chemisorption of H on magnetic Ni(001). <i>Physical Review Letters</i> , 1985 , 54, 1547-1550	7.4	98
200	Image planes and surface states. <i>Physical Review Letters</i> , 1985 , 55, 2055-2058	7.4	91
199	Pairing of $j=3/2$ Fermions in Half-Heusler Superconductors. <i>Physical Review Letters</i> , 2016 , 116, 177001	7.4	88
198	Stacking faults in magnesium. <i>Physical Review B</i> , 1997 , 56, 10844-10851	3.3	87
197	Structure of the hydrogen-stabilized MgO(111) $\overline{1}\overline{1}\overline{1}$ polar surface: Integrated experimental and theoretical studies. <i>Physical Review B</i> , 2005 , 71,	3.3	83
196	Spiral growth without dislocations: molecular beam epitaxy of the topological insulator Bi ₂ Se ₃ on epitaxial graphene/SiC(0001). <i>Physical Review Letters</i> , 2012 , 108, 115501	7.4	81
195	Direct experimental determination of onset of electron-electron interactions in gap opening of zigzag graphene nanoribbons. <i>Nature Communications</i> , 2014 , 5, 4311	17.4	74
194	Evidence of nanocrystalline semiconducting graphene monoxide during thermal reduction of graphene oxide in vacuum. <i>ACS Nano</i> , 2011 , 5, 9710-7	16.7	73
193	Unoccupied surface states on Cu(001): A comparison of experiment and theory. <i>Physical Review B</i> , 1986 , 33, 760-764	3.3	72

192	Exploring Adsorption and Reactivity of NH ₃ on Reduced Graphene Oxide. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 10698-10707	3.8	70
191	Ag nanocrystal as a promoter for carbon nanotube-based room-temperature gas sensors. <i>Nanoscale</i> , 2012 , 4, 5887-94	7.7	68
190	Structural instabilities of excited phases. <i>Physical Review B</i> , 1997 , 55, 787-797	3.3	67
189	FLAPW: applications and implementations. <i>Journal of Physics Condensed Matter</i> , 2009 , 21, 084201	1.8	66
188	Unusual adsorption site of hydrogen on the unreconstructed Ir(100) surface. <i>Physical Review B</i> , 2006 , 73,	3.3	64
187	Linear augmented Slater-type-orbital study of Au-5d-transition-metal alloying. <i>Physical Review B</i> , 1987 , 35, 508-518	3.3	64
186	Revealing the substrate origin of the linear dispersion of silicene/Ag(111). <i>Nano Letters</i> , 2014 , 14, 5189-91.5	3.5	63
185	Requirements for the formation of a chiral template. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 851-6	3.4	63
184	Magnetism of linear chains. <i>Journal of Magnetism and Magnetic Materials</i> , 1983 , 38, 23-33	2.8	63
183	Vacancy formation energies of fcc transition metals calculated by a full potential green's function method. <i>Solid State Communications</i> , 1991 , 79, 31-35	1.6	62
182	Spin-polarized photoemission studies of the adsorption of O and S on Fe(001). <i>Physical Review B</i> , 1990 , 41, 9659-9667	3.3	62
181	Stability of Zr-Al alloys. <i>Physical Review B</i> , 1998 , 57, R2009-R2012	3.3	61
180	High-resolution inverse-photoemission study of the Pd(111) surface. <i>Physical Review B</i> , 1986 , 34, 3670-3673	3.3	61
179	Full-potential linear augmented-Slater-type-orbital method. <i>Physical Review B</i> , 1989 , 40, 2757-2766	3.3	60
178	Relativistic spin polarization and magnetization: Knight shift of Pt(001). <i>Physical Review B</i> , 1983 , 28, 6263-6269	3.59	59
177	Electronic structure of the (2 x 2)C rho 4g carbidic phase on Ni{100}. <i>Physical Review B</i> , 1986 , 34, 2199-2206	3.5	58
176	Contributions to the work function of crystals. <i>Physical Review B</i> , 1984 , 29, 3001-3008	3.3	57
175	Adsorbed layer and multilayer materials: The energetics and bonding of Pd and Ag on Nb(001) and Nb(110). <i>Physical Review B</i> , 1989 , 39, 12585-12597	3.3	55

174	Enthalpies of formation of AlNi: Experiment versus theory. <i>Journal of Phase Equilibria and Diffusion</i> , 1998 , 19, 106-111		53
173	Role of defect sites and Ga polarization in the magnetism of Mn-doped GaN. <i>Physical Review Letters</i> , 2005 , 95, 257201	7-4	49
172	First-principles study of titanium oxides. <i>Physical Review B</i> , 1996 , 54, 7857-7864	3-3	49
171	Linear augmented-Slater-type-orbital method for electronic-structure calculations. V. Spin-orbit splitting in Cu ₃ Au. <i>Physical Review B</i> , 1988 , 37, 9985-9992	3-3	48
170	First-principles calculation of the activation energy for diffusion in liquid sodium. <i>Physical Review Letters</i> , 1990 , 64, 1146-1149	7-4	46
169	Designing substrates for silicene and germanene: First-principles calculations. <i>Physical Review B</i> , 2016 , 94,	3-3	46
168	Enthalpies of formation of Ni ₃ Al: Experiment versus theory. <i>Journal of Phase Equilibria and Diffusion</i> , 1996 , 17, 173-178		45
167	H and W(001) surface reconstructions: Local bonding to surface states. <i>Physical Review Letters</i> , 1986 , 56, 2295-2298	7-4	45
166	Magnetic surface states on Fe(001). <i>Physical Review B</i> , 1990 , 41, 2643-2645	3-3	44
165	Electric-field-induced modification of the magnon energy, exchange interaction, and curie temperature of transition-metal thin films. <i>Physical Review Letters</i> , 2015 , 114, 107202	7-4	43
164	First-principles molecular dynamics for metals. <i>Physical Review B</i> , 1989 , 40, 7985-7988	3-3	43
163	Spatial fluctuations in barrier height at the graphene-silicon carbide Schottky junction. <i>Nature Communications</i> , 2013 , 4, 2752	17-4	42
162	Linear augmented-Slater-type-orbital method for electronic-structure calculations. III. Structural and cohesive energies of the 5d elements Lu-Au. <i>Physical Review B</i> , 1985 , 32, 4883-4891	3-3	42
161	Theoretical 2p-core-level shift and crystal-field splitting at the Al(001) surface. <i>Physical Review B</i> , 1981 , 24, 2292-2294	3-3	42
160	Electronic structure of Au and Ag overlayers on Ru(001): The behavior of the noble-metal d bands. <i>Physical Review B</i> , 1995 , 51, 9979-9984	3-3	40
159	Phase transitions in a mercury monolayer. <i>Physical Review B</i> , 1983 , 28, 593-597	3-3	40
158	Force constants for substitutional alloys. <i>Physical Review B</i> , 1999 , 59, 4100-4111	3-3	38
157	Cohesion and lattice stabilities in the 5d transition metals: Full versus muffin-tin potentials. <i>Physical Review B</i> , 1990 , 41, 11813-11821	3-3	38

156	Contribution of electronic excitations to the entropy of crystals: The relative stabilities of the hcp, fcc, and bcc structures among the transition metals. <i>Physical Review B</i> , 1984 , 30, 1641-1645	3-3	38
155	Layer k-projection and unfolding electronic bands at interfaces. <i>Physical Review B</i> , 2018 , 98,	3-3	38
154	Spin-orbit interactions and the nematicity observed in the fe-based superconductors. <i>Physical Review Letters</i> , 2015 , 114, 167001	7-4	36
153	Constraint density functional calculations for multiplets in a ligand-field applied to Fe-phthalocyanine. <i>Physical Review B</i> , 2012 , 85,	3-3	36
152	Creation of Low-Coordination Gold Sites on Au(111) Surface by 1,4-phenylene Diisocyanide Adsorption. <i>Topics in Catalysis</i> , 2011 , 54, 20-25	2-3	35
151	Selected growth of cubic and hexagonal GaN epitaxial films on polar MgO(111). <i>Physical Review Letters</i> , 2005 , 94, 216101	7-4	35
150	Resilient Nodeless d-Wave Superconductivity in Monolayer FeSe. <i>Physical Review Letters</i> , 2017 , 119, 267001	7-4	34
149	Angle-resolved positronium emission spectroscopy. <i>Physical Review Letters</i> , 1987 , 58, 921-924	7-4	32
148	Linear augmented-Slater-type-orbital method for electronic-structure calculations. II. bcc, fcc, and hcp W. <i>Physical Review B</i> , 1985 , 32, 4876-4882	3-3	32
147	Si diffusion path for pit-free graphene growth on SiC(0001). <i>Physical Review B</i> , 2011 , 84,	3-3	31
146	Spin-resolved photoemission study of photohole lifetimes in ferromagnetic gadolinium. <i>Physical Review B</i> , 2002 , 65,	3-3	31
145	Comment on "Ferromagnetism of the Rh(001) surface". <i>Physical Review Letters</i> , 1993 , 71, 4097	7-4	31
144	Localized states at metal-metal interfaces: An inverse photoemission study of Pd/Nb(110). <i>Physical Review B</i> , 1988 , 38, 7850-7853	3-3	31
143	Surface electronic structure and off-site Auger transitions on TaC(111) observed with Auger-photoelectron coincidence spectroscopy. <i>Physical Review Letters</i> , 1992 , 68, 2247-2250	7-4	30
142	Observation of surface to bulk interatomic Auger decay from Ta(100). <i>Physical Review B</i> , 1990 , 41, 12468-12473	3-3	30
141	A statistical thermodynamics model for monolayer gas adsorption on graphene-based materials: implications for gas sensing applications. <i>RSC Advances</i> , 2014 , 4, 47481-47487	3-7	29
140	Magnetism on the surface of the bulk paramagnetic intermetallic compound YCo ₂ . <i>Physical Review Letters</i> , 2005 , 94, 146403	7-4	29
139	Ternary transition-metal aluminide alloy formation: The BiF ₃ structure. <i>Physical Review B</i> , 1998 , 57, 12134-12138	3-3	28

138	Comment on "Structure of Au(100)". <i>Physical Review Letters</i> , 1987 , 58, 1382	7.4	28
137	Local-density approximation: Cohesion in the transition metals and s \rightarrow d promotion in the transition-metal atoms. <i>Physical Review B</i> , 1991 , 43, 1455-1462	3.3	27
136	Hyperfine fields at surfaces and interfaces. <i>Hyperfine Interactions</i> , 1987 , 33, 53-68	0.8	27
135	Dynamically stabilized growth of polar oxides: the case of MgO(111). <i>Physical Review Letters</i> , 2011 , 107, 056101	7.4	26
134	Atomic and electronic structure of the Fe ₃ O ₄ (111)/MgO(111) model polar oxide interface. <i>Physical Review B</i> , 2005 , 72,	3.3	26
133	Charge transfer in gold-alkali-metal systems. <i>Physical Review B</i> , 1994 , 49, 7148-7154	3.3	26
132	Energetics of transition-metal alloy formation: Ti, Zr, and Hf alloyed with the heavier 4d and 5d elements. <i>Physical Review B</i> , 1989 , 39, 10761-10769	3.3	26
131	Electric-field gradients in dilute Cu alloys: The role of the Cu d electrons. <i>Physical Review B</i> , 1990 , 42, 9336-9339	3.3	25
130	Linear augmented Slater-type orbital study of Pt-5d-transition-metal alloying. <i>Physical Review B</i> , 1987 , 36, 6396-6410	3.3	25
129	Vibrational Excitations and Low Energy Electronic Structure of Epoxide-decorated Graphene. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 212-219	6.4	24
128	Interaction of helium with a graphite surface. <i>Surface Science</i> , 1984 , 145, 207-222	1.8	24
127	Magnetic Energy Anomalies of 3 d Systems. <i>Europhysics Letters</i> , 1993 , 24, 495-500	1.6	23
126	Linear augmented-Slater-type-orbital method for electronic-structure calculations. IV. 5d-5d alloys. <i>Physical Review B</i> , 1986 , 34, 8421-8429	3.3	23
125	Structure of Methyl Pyruvate and π (1-Naphthyl)ethylamine on Pd(111). <i>Journal of Physical Chemistry C</i> , 2011 , 115, 8790-8797	3.8	22
124	Charging Dirac states at antiphase domain boundaries in the three-dimensional topological insulator Bi ₂ Se ₃ . <i>Physical Review Letters</i> , 2013 , 110, 186804	7.4	21
123	Final-state screening of core holes in metals. <i>Physical Review B</i> , 1986 , 34, 2971-2974	3.3	21
122	Enthalpies of formation of AlFe: Experiment versus theory. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2000 , 24, 309-318	1.9	20
121	Strain-induced band-gap engineering of graphene monoxide and its effect on graphene. <i>Physical Review B</i> , 2013 , 87,	3.3	19

120	YCo2: intrinsic magnetic surface of a paramagnetic bulk material. <i>Physical Review Letters</i> , 2007 , 99, 047204	4	19
119	Magnetic moment of iron in metallic environments. <i>Physical Review B</i> , 2000 , 61, 375-381	3.3	19
118	Thickness Induced Buckling of bcc Copper Films. <i>Physical Review Letters</i> , 1999 , 83, 780-783	7.4	19
117	Electric-field-induced changes in scanning tunneling microscopy images of metal surfaces. <i>Chemical Physics Letters</i> , 1999 , 315, 167-172	2.5	19
116	Charge transfer in transition-metal alloying: Charge-tailing effects. <i>Physical Review B</i> , 1991 , 43, 1446-1454	3.3	19
115	The energetics of transition metal alloy formation: Theory versus experiment. <i>Scripta Metallurgica</i> , 1988 , 22, 1285-1289		19
114	Evidence for d-Wave Superconductivity in Single Layer FeSe/SrTiO Probed by Quasiparticle Scattering Off Step Edges. <i>Nano Letters</i> , 2019 , 19, 2497-2502	11.5	18
113	Magnetic fluctuations in single-layer FeSe. <i>Communications Physics</i> , 2018 , 1,	5.4	18
112	Excited Cr impurity states in Al ₂ O ₃ from constraint density functional theory. <i>Physical Review B</i> , 2013 , 87,	3.3	18
111	Electronic structure and thermodynamics of defects in NiAl ₃ . <i>Physical Review B</i> , 2001 , 64,	3.3	18
110	Determination of the elastic tensor in low-symmetry structures. <i>Europhysics Letters</i> , 1998 , 43, 183-188	1.6	18
109	Heats of formation of transition-metal alloys: Full-potential approach and the Pt-Ti system. <i>Physical Review B</i> , 1992 , 45, 8233-8238	3.3	18
108	Two-dimensional angular correlation of annihilation radiation study of positron interactions with surfaces of aluminum. <i>Physical Review B</i> , 1989 , 39, 3966-3989	3.3	18
107	Magnetism at surfaces and interfaces. <i>Journal of Magnetism and Magnetic Materials</i> , 1983 , 38, 269-272	2.8	18
106	Strain and structure driven complex magnetic ordering of a CoO overlayer on Ir(100). <i>Physical Review Letters</i> , 2012 , 109, 015501	7.4	17
105	Incommensurate Moiré overlayer with strong local binding: CoO(111) bilayer on Ir(100). <i>Physical Review B</i> , 2012 , 86,	3.3	17
104	Transition-metal aluminide formation: The 4d aluminides. <i>Physical Review B</i> , 2001 , 65,	3.3	17
103	Surface resonances on Ta(001). <i>Physical Review B</i> , 1990 , 42, 5025-5039	3.3	17

102	Stabilizing the spin vortex crystal phase in two-dimensional iron-based superconductors. <i>Physical Review B</i> , 2017 , 95,	3.3	17
101	Indirect Interlayer Bonding in Graphene-Topological Insulator van der Waals Heterostructure: Giant Spin-Orbit Splitting of the Graphene Dirac States. <i>ACS Nano</i> , 2016 , 10, 8450-6	16.7	17
100	Anisotropic thermal conductivity of semiconducting graphene monoxide. <i>Applied Physics Letters</i> , 2013 , 102, 223101	3.4	16
99	Effects of magnetic dopants in (Li _{0.8} M _{0.2} OH)FeSe (M=Fe, Mn, Co): Density functional theory study using a band unfolding technique. <i>Physical Review B</i> , 2017 , 96,	3.3	16
98	Potassium adsorption and an unoccupied surface state on Fe(001). <i>Journal of Physics Condensed Matter</i> , 1998 , 10, 95-100	1.8	16
97	A comparison of the surface electronic structure of Ta(100) and TaC(111) using Auger-photoelectron coincidence spectroscopy. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1991 , 9, 1919-1923	2.9	16
96	Half-metallic Dirac cone in zigzag graphene nanoribbons on graphene. <i>Physical Review B</i> , 2016 , 94,	3.3	16
95	Observation of orbital angular momentum in the chiral magnet CrNb ₃ S ₆ by soft x-ray magnetic circular dichroism. <i>Physical Review B</i> , 2019 , 99,	3.3	14
94	Structure determination of disordered organic molecules on surfaces from the Bragg spots of low-energy electron diffraction and total energy calculations. <i>Physical Review B</i> , 2004 , 69,	3.3	14
93	On the Pressure Dependence of Shear Strengths in Sliding, Boundary-Layer Friction. <i>Tribology Letters</i> , 2011 , 44, 67-73	2.8	13
92	Electronic structures of Mn-induced phases on GaN(0001). <i>Physical Review B</i> , 2009 , 80,	3.3	13
91	Atomistic view of the autosurfactant effect during GaN epitaxy. <i>Physical Review Letters</i> , 2007 , 98, 206106.	6.4	13
90	XANES study of hydrogen incorporation in a Pd-capped Nb thin film. <i>Physical Review B</i> , 1998 , 57, 3881-3886	3.3	13
89	Interplay of paramagnetism and topology in the Fe-chalcogenide high-T _c superconductors. <i>Physical Review B</i> , 2019 , 99,	3.3	12
88	X-ray absorption near-edge structure analysis of the chemical environment of zinc in the tribological film formed by zinc dialkyl dithiophosphate decomposition on steel. <i>Tribology International</i> , 2005 , 38, 195-204	4.9	12
87	Transition-metals and their alloys. <i>Solid State Physics</i> , 2001 , 56, 1-112	2	12
86	Reversible depression in the T _c of thin Nb films due to enhanced hydrogen adsorption. <i>Physical Review B</i> , 1998 , 58, 6585-6590	3.3	12
85	A Convergence Test of the Full-potential Linearized Augmented Plane Wave (FLAPW) Method: Ferromagnetic Bulk BCC Fe. <i>Journal of Magnetism</i> , 2009 , 14, 137-143	1.9	12

84	Formation of nitrogen-vacancy complexes during plasma-assisted nitrogen doping of epitaxial graphene on SiC(0001). <i>Applied Physics Letters</i> , 2012 , 100, 233119	3.4	11
83	Cu/Pd multilayers: An atomistic structural study. <i>Physical Review B</i> , 1993 , 47, 13636-13642	3.3	11
82	Surface electronic structure of GaAs(110) studied by Auger photoelectron coincidence spectroscopy. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1991 , 9, 1907-1912	2.9	11
81	Self-consistent FLAPW determination of surface magnetism: Fe(001). <i>Journal of Magnetism and Magnetic Materials</i> , 1983 , 31-34, 889-890	2.8	11
80	Spin-Polarized Band-Structure Determination of the Si ₂ Molecular Ground State by the Method of Full-Potential Linearized Augmented Plane Waves. <i>Physical Review Letters</i> , 1981 , 47, 705-708	7.4	11
79	Investigation of NO ₂ adsorption on reduced graphene oxide. <i>Chemical Physics Letters</i> , 2015 , 622, 86-91	2.5	10
78	Electric-field-driven hole carriers and superconductivity in diamond. <i>Physical Review B</i> , 2013 , 87,	3.3	10
77	Dielectric constant of NiO and LDA+U. <i>Physical Review B</i> , 2013 , 87,	3.3	10
76	First-principles calculations of the self-trapped exciton in crystalline NaCl. <i>Physical Review B</i> , 2000 , 62, 12589-12592	3.3	10
75	Antiferromagnetism of CuO ₂ layers. <i>Physical Review B</i> , 1989 , 39, 835-838	3.3	10
74	Effects of interface oxygen vacancies on electronic bands of FeSe/SrTiO ₃ (001). <i>Physical Review B</i> , 2016 , 94,	3.3	10
73	Termination-dependent edge states of MBE-grown WSe ₂ . <i>Physical Review B</i> , 2018 , 98,	3.3	10
72	Determining charge state of graphene vacancy by noncontact atomic force microscopy and first-principles calculations. <i>Nanotechnology</i> , 2015 , 26, 035702	3.4	9
71	Shear properties of potassium chloride films on iron obtained using density functional theory. <i>Journal of Physics Condensed Matter</i> , 2011 , 23, 265003	1.8	9
70	Role of functionalized transition-metal coated W tips in STM imaging: Application to epitaxial graphene on SiC(0001). <i>Physical Review B</i> , 2011 , 84,	3.3	9
69	Giant Coster-Kronig transitions and intrinsic line shapes of the anomalous Pd M45VV Auger spectrum of Pd/Ag(100) dilute surface alloys. <i>Physical Review Letters</i> , 2003 , 91, 176403	7.4	9
68	Local atomic environments in periodic and aperiodic Al-Mn alloys. <i>Physical Review B</i> , 1986 , 34, 8270-8273	3.3	9
67	Structural stabilities of layered materials: Pt-Ta. <i>Physical Review B</i> , 1987 , 35, 9284-9286	3.3	9

66	Search for the ground-state electronic configurations of correlated organometallic metallocenes from constraint density functional theory. <i>Physical Review B</i> , 2016 , 94,	3.3	8
65	STEM and EELS study of the Graphene/Bi ₂ Se ₃ Interface. <i>Microscopy and Microanalysis</i> , 2015 , 21, 1151-1153		8
64	Atomic and electronic structure of polar Fe ₂ O ₃ (0001)/MgO(111) interfaces. <i>Physical Review B</i> , 2012 , 86,	3.3	8
63	Electron standing waves on the GaN(0001)-pseudo (1 × 1) surface: a FT-STM study at room temperature. <i>Nanotechnology</i> , 2010 , 21, 435401	3.4	8
62	On the role of classical and quantum notions in channeling and the development of fast positrons as a solid state probe of valence electron and spin densities. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1996 , 119, 30-41	1.2	8
61	All-electron self-consistent determination of spin-polarization and knight shift of A Pt(001)film. <i>Journal of Magnetism and Magnetic Materials</i> , 1983 , 31-34, 891-892	2.8	8
60	Cohesive and Structural Energies for the 5dElements, Lu through Au. <i>Physica Scripta</i> , 1985 , 32, 425-428	2.6	8
59	Topological band and superconductivity in UTe ₂ . <i>Physical Review B</i> , 2021 , 103,	3.3	8
58	Scaled effective on-site Coulomb interaction in the DFT+U method for correlated materials. <i>Physical Review B</i> , 2018 , 97,	3.3	7
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