Peter Kratzer

List of Publications by Year
in descending order

150 papers	5,286 citations	66343 42 h-index	98798 67 g-index
152 all docs	152 docs citations	152 times ranked	4393 citing authors

#	Article	IF	Citations
1	A theoretical study of CH4 dissociation on pure and goldâ€alloyed Ni(111) surfaces. Journal of Chemical Physics, 1996, 105, 5595-5604.	3.0	262
2	Preserving the Half-Metallicity at the Heusler AlloyCo2MnSi(001)Surface: A Density Functional Theory Study. Physical Review Letters, 2005, 94, 096402.	7.8	167
3	Effect of the cluster size in modeling the H2 desorption and dissociative adsorption on Si(001). Journal of Chemical Physics, 1999, 110, 3986-3994.	3.0	162
4	Atomic Structure of theGaAs(001)â^'(2Ã—4)Surface Resolved Using Scanning Tunneling Microscopy and First-Principles Theory. Physical Review Letters, 1999, 83, 2989-2992.	7.8	159
5	Formation and Stability of Self-Assembled Coherent Islands in Highly Mismatched Heteroepitaxy. Physical Review Letters, 1999, 82, 4042-4045.	7.8	147
6	Role of Electronic Correlation in the Si(100) Reconstruction: A Quantum Monte Carlo Study. Physical Review Letters, 2001, 87, 016105.	7.8	146
7	Magnetism in C- or N-doped MgO and ZnO: A Density-Functional Study of Impurity Pairs. Physical Review Letters, 2010, 105, 267203.	7.8	111
8	Geometric and electronic factors determining the differences in reactivity of H2 on Cu(100) and Cu(111). Surface Science, 1996, 359, 45-53.	1.9	100
9	Highly Site-SpecificH2Adsorption on VicinalSi(001)Surfaces. Physical Review Letters, 1998, 81, 5596-5599.	7.8	100
10	Size, shape, and stability of InAs quantum dots on the GaAs(001) substrate. Physical Review B, 2000, 62, 1897-1904.	3.2	96
11	Probing Interface Electronic Structure with Overlayer Quantum-Well Resonances:Al/Si(111). Physical Review Letters, 2001, 87, 156801.	7.8	95
12	Highly excited molecules from Eley-Rideal reactions. Surface Science, 1991, 254, 275-280.	1.9	93
13	Effect of strain on surface diffusion in semiconductor heteroepitaxy. Physical Review B, 2001, 64, .	3.2	92
14	Reaction-Limited Island Nucleation in Molecular Beam Epitaxy of Compound Semiconductors. Physical Review Letters, 2002, 88, 036102.	7.8	88
15	Reaction dynamics of atomic hydrogen with the hydrogenated Si(001) (2Ã—1) surface. Journal of Chemical Physics, 1997, 106, 6752-6763.	3.0	87
16	First-principles studies of kinetics in epitaxial growth of III-V semiconductors. Applied Physics A: Materials Science and Processing, 2002, 75, 79-88.	2.3	86
17	Direct pathway for sticking/desorption ofH2on Si(100). Physical Review B, 1995, 51, 13432-13440.	3.2	84
18	Arsenic Dimer Dynamics during MBE Growth: Theoretical Evidence for a Novel Chemisorption State ofAs2Molecules on GaAs Surfaces. Physical Review Letters, 1999, 82, 4886-4889.	7.8	83

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19	Quantum Monte Carlo Calculations ofH2Dissociation on Si(001). Physical Review Letters, 2002, 89, 166102.	7.8	83
20	Tight-binding study of the influence of the strain on the electronic properties of InAs/GaAs quantum dots. Physical Review B, 2003, 68, .	3.2	81
21	Shape transition during epitaxial growth ofInAsquantum dots onGaAs(001): Theory and experiment. Physical Review B, 2006, 73, .	3.2	80
22	Electronic and Structural Differences between Wurtzite and Zinc Blende InAs Nanowire Surfaces: Experiment and Theory. ACS Nano, 2014, 8, 12346-12355.	14.6	78
23	Designing surface alloys with specific active sites. Catalysis Letters, 1996, 40, 131-135.	2.6	77
24	Understanding the growth mechanisms of GaAs and InGaAs thin films by employing first-principles calculations. Applied Surface Science, 2003, 216, 436-446.	6.1	77
25	Reaction dynamics of molecular hydrogen on silicon surfaces. Physical Review B, 1996, 54, 5978-5991.	3.2	75
26	Density-Functional Theory Study of Half-Metallic Heterostructures: Interstitial Mn in Si. Physical Review Letters, 2007, 98, 117202.	7.8	71
27	Thermodynamics of the Heusler alloy<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Co</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>MnSi. A combined density functional theory and cluster expansion s. Physical Review B, 2009, 79, .	3.2	67
28	First-Principles Study of Ferromagnetism in Epitaxial Si-Mn Thin Films on Si(001). Physical Review Letters, 2004, 92, 237202.	7.8	66
29	Ordering of the Nanoscale Step Morphology As a Mechanism for Droplet Self-Propulsion. Nano Letters, 2009, 9, 2710-2714.	9.1	66
30	The coupling between adsorption dynamics and the surface structure: H2 on Si(100). Chemical Physics Letters, 1994, 229, 645-649.	2.6	65
31	Control of fine-structure splitting and excitonic binding energies in selected individual InAsâˆ•GaAs quantum dots. Applied Physics Letters, 2006, 89, 263109.	3.3	60
32	Direct Atomic Scale Imaging of IIIâˆ’V Nanowire Surfaces. Nano Letters, 2008, 8, 3978-3982.	9.1	59
33	Analytic many-body potential for InAs/GaAs surfaces and nanostructures: Formation energy of InAs quantum dots. Physical Review B, 2008, 77, .	3.2	57
34	The Basics of Electronic Structure Theory for Periodic Systems. Frontiers in Chemistry, 2019, 7, 106.	3.6	57
35	First-principles study of spin-dependent thermoelectric properties of half-metallic Heusler thin films between platinum leads. Physical Review B, 2014, 89, .	3.2	56
36	Epitaxy of Mn on Si(001): Adsorption, surface diffusion, and magnetic properties studied by density-functional theory. Physical Review B, 2006, 74, .	3.2	54

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37	Calculation of the diameter-dependent polytypism in GaAs nanowires from an atomic motif expansion of the formation energy. Physical Review B, 2011, 84, .	3.2	53
38	Anisotropic diffusion of In adatoms on pseudomorphicInxGa1âˆ'xAsfilms: First-principles total energy calculations. Physical Review B, 2004, 69, .	3.2	52
39	GaAs(2511): A New Stable Surface within the Stereographic Triangle. Physical Review Letters, 2001, 86, 3815-3818.	7.8	49
40	Model for nucleation in GaAs homoepitaxy derived from first principles. Physical Review B, 1999, 59, 15246-15252.	3.2	47
41	Exchange interactions and critical temperature of bulk and thin films of MnSi: A density functional theory study. Physical Review B, 2008, 78, .	3.2	46
42	First-principles study of thin magnetic transition-metal silicide films on Si(001). Physical Review B, 2005, 72, .	3.2	45
43	Band structure and thermoelectric properties of half-Heusler semiconductors from many-body perturbation theory. Physical Review B, 2018, 97, .	3.2	43
44	Hydrogen vibrational modes on graphene and relaxation of the Câ€“H stretch excitation from first-principles calculations. Journal of Chemical Physics, 2010, 133, 054505.	3.0	40
45	Atomic Structure of theGaAs(001)âˆ'c(4Ã—4)Surface: First-Principles Evidence For Diversity of Heterodimer Motifs. Physical Review Letters, 2004, 93, 146102.	7.8	39
46	Structural Stability and Magnetic and Electronic Properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Co</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>MnSi</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>001</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 372 Td (stretchy="false")</mml:mo>	7.8	37
47	A Density-Functional Theory Study. Physical Review Letters, 2009, 103, 046802. Elastic response of cubic crystals to biaxial strain: Analytic results and comparison to density functional theory for InAs. Physical Review B, 2007, 75, .	3.2	35
48	Density-functional study of hydrogen chemisorption on vicinal Si(001) surfaces. Physical Review B, 1999, 59, 2790-2800.	3.2	34
49	Growth mode and atomic structure of MnSi thin films on Si(111). Physical Review B, 2012, 86, .	3.2	33
50	Reduced thermal conductivity of TiNiSn/HfNiSn superlattices. Physical Review B, 2015, 92, .	3.2	33
51	Ternary semiconductors NiZrSn and CoZrBi with half-Heusler structure: A first-principles study. Physical Review B, 2016, 94, .	3.2	32
52	Ab initio quantum dynamics of adsorption/desorption on a 3-D potential. Surface Science, 1996, 345, 125-137.	1.9	31
53	Electron-hole spectra created by adsorption on metals from density functional theory. Physical Review B, 2009, 79, .	3.2	31
54	Anisotropic ferromagnetism in carbon-doped zinc oxide from first-principles studies. Physical Review B, 2012, 86, .	3.2	31

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55	D2 dissociative adsorption on and associative desorption from Si(100): Dynamic consequences of an ab initio potential energy surface. Journal of Chemical Physics, 1996, 104, 3075-3091.	3.0	30
56	InAs quantum dots grown on theGaAs(113)AandGaAs(1Â¯1Â¯3Â¯)Bsurfaces: A comparative STM study. Physical Review B, 2003, 68, .	3.2	30
57	Density-functional study of Mn monosilicide on the Si(111) surface: Film formation versus island nucleation. Physical Review B, 2007, 76, .	3.2	30
58	Catalytic Role of Gold Nanoparticle in GaAs Nanowire Growth: A Density Functional Theory Study. Nano Letters, 2012, 12, 943-948.	9.1	30
59	Indium surface diffusion on InAs<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>2</mml:mn><mml:mo>Ã—</mml:mo><mm wetting layers on GaAs(001). Physical Review B, 2009, 79, .	3.2	29
60	Spincaloric properties of epitaxial<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Co</mml:mi><mml:mn>2</mml:mn></mml: tunnel junctions. Physical Review B, 2015, 92, .	3.2	29
61	Atomic Structure of the Stoichiometric GaAs(114) Surface. Physical Review Letters, 2001, 86, 115-118.	7.8	28
62	Electronic structure changes ofSi(001)â^’(2Ã—1)from subsurface Mn observed by STM. Physical Review B, 2007, 75, .	3.2	28
63	Two-dimensional electron gases: Theory of ultrafast dynamics of electron-phonon interactions in graphene, surfaces, and quantum wells. Journal of Applied Physics, 2009, 105, 122409.	2.5	28
64	Island dissolution during capping layer growth interruption. Applied Physics A: Materials Science and Processing, 2001, 73, 161-165.	2.3	27
65	Density-functional theory study of vibrational relaxation of CO stretching excitation on Si(100). Journal of Chemical Physics, 2008, 129, 174702.	3.0	27
66	As vacancies, Ga antisites, and Au impurities in zinc blende and wurtzite GaAs nanowire segments from first principles. Physical Review B, 2013, 87, .	3.2	27
67	The dynamics of the H + D/Si(001) reaction: a trajectory study based on ab initio potentials. Chemical Physics Letters, 1998, 288, 396-402.	2.6	26
68	Thermoelectric transport in periodic one-dimensional stacks of InAs/GaAs quantum dots. Physical Review B, 2010, 82, .	3.2	26
69	Chemisorption and Physisorption at the Metal/Organic Interface: Bond Energies of Naphthalene and Azulene on Coinage Metal Surfaces. Journal of Physical Chemistry C, 2020, 124, 8257-8268.	3.1	26
70	Role of sidewall diffusion in GaAs nanowire growth: A first-principles study. Physical Review B, 2012, 86, .	3.2	25
71	Surface structure of GaAs(2 5 11). Physical Review B, 2002, 65, .	3.2	24
72	Density functional study of carbon doping in ZnO. Semiconductor Science and Technology, 2011, 26, 014038.	2.0	24

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73	Native defects in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Co</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>Z</mml:mi></mml:mrow></mml:math> full Heusler alloys: Formation and. Physical Review B, 2017, 96, .	3.2	24
74	Density-functional theory studies on microscopic processes of gaas growth. Progress in Surface Science, 1998, 59, 135-147.	8.3	22
75	Surface knowledge: toward a predictive theory of materials. Computing in Science and Engineering, 2001, 3, 16-25.	1.2	21
76	Atomistic modeling of the Au dropletâ€“GaAs interface for size-selective nanowire growth. Physical Review B, 2013, 88, .	3.2	21
77	Au wetting and nanoparticle stability on GaAs(111)B. Applied Physics Letters, 2006, 89, 251912.	3.3	20
78	Moleculeâ€“Metal Bond of Alternant versus Nonalternant Aromatic Systems on Coinage Metal Surfaces: Naphthalene versus Azulene on Ag(111) and Cu(111). Journal of Physical Chemistry C, 2019, 123, 29219-29230.	3.1	20
79	Interplay of growth mode and thermally induced spin accumulation in epitaxial<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>Al/Co</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:mi>Z</mml:mi></mml:math> Physical Review B, 2014, 89, .	3.2	19
80	Commensurate versus incommensurate heterostructures of group-III monochalcogenides. Physical Review Materials, 2018, 2, .	2.4	19
81	Analytic many-body potential for GaAs(001) homoepitaxy: Bulk and surface properties. Physical Review B, 2011, 83, .	3.2	18
82	Energetics of InAs Thin Films and Islands on the GaAs(001) Substrate. Japanese Journal of Applied Physics, 2000, 39, 4298-4301.	1.5	17
83	In adatom diffusion on In_xGa_{1â^'x}As/GaAs(001): effects of strain, reconstruction and composition. Journal of Physics Condensed Matter, 2009, 21, 355007.	1.8	16
84	Strain stabilization and thickness dependence of magnetism in epitaxial transition metal monosilicide thin films on Si(111). Physical Review B, 2013, 88, .	3.2	16
85	Mode conversion and long-lived vibrational modes in lead monolayers on silicon (111) after femtosecond laser excitation: A molecular dynamics simulation. Physical Review B, 2013, 88, .	3.2	15
86	Indium coverage of the Si(111)- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msqrt><mml:mn>7</mml:mn></mml:msqrt><mml:mo>Ã—</mml:mo></mml:mrow></mml:math> -In surface. Physical Review B, 2017, 96, .	3.2	15
87	Transition-metal silicides as materials for magnet-semiconductor heterostructures. Journal of Applied Physics, 2007, 101, 081725.	2.5	14
88	Effect of post-growth annealing on the optical properties of InAs/GaAs quantum dots: A tight-binding study. Journal of Applied Physics, 2007, 102, 023711.	2.5	14
89	Adsorption of indium on an InAs wetting layer deposited on the GaAs(001) surface. Physical Review B, 2008, 77, .	3.2	14
90	Searching for Si-based spintronics by first principles calculations. New Journal of Physics, 2009, 11, 125009.	2.9	14

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91	Crystal Structure Induced Preferential Surface Alloying of Sb on Wurtzite/Zinc Blende GaAs Nanowires. Nano Letters, 2017, 17, 3634-3640.	9.1	14
92	All-electron real-time and imaginary-time time-dependent density functional theory within a numeric atom-centered basis function framework. Journal of Chemical Physics, 2021, 155, 154801.	3.0	14
93	Isotope effects in the vibrational lifetime of hydrogen on germanium(100): Theory and experiment. Journal of Chemical Physics, 2009, 131, 124502.	3.0	13
94	Electronic excitations in magnesium epitaxy: Experiment and theory. Physical Review B, 2010, 82, .	3.2	13
95	Comparison of density functionals for nitrogen impurities in ZnO. Journal of Chemical Physics, 2013, 138, 234702.	3.0	13
96	Magnetic monolayer Li 2 N: Density Functional Theory calculations. Europhysics Letters, 2017, 119, 57002.	2.0	13
97	Spin caloric transport from density-functional theory. Journal Physics D: Applied Physics, 2019, 52, 073001.	2.8	13
98	Large Seebeck magnetic anisotropy in thin Co films embedded in Cu determined byab initioinvestigations. Physical Review B, 2013, 88, .	3.2	12
99	Structure and morphology of the As-rich and the stoichiometric GaAs(114)A surface. Journal of Applied Physics, 2004, 95, 7645-7654.	2.5	11
100	The role of the van der Waals interactions in the adsorption of anthracene and pentacene on the Ag(111) surface. Journal of Chemical Physics, 2017, 146, 034702.	3.0	11
101	Enhanced electronic and magnetic properties by functionalization of monolayer GaS via substitutional doping and adsorption. Journal of Physics Condensed Matter, 2018, 30, 195805.	1.8	11
102	Signatures of the Dichalcogenideâ€“Gold Interaction in the Vibrational Spectra of MoS₂ and MoSe₂ on Au(111). Journal of Physical Chemistry C, 2021, 125, 26645-26651.	3.1	11
103	First-principles computational exploration of ferromagnetism in monolayer GaS via substitutional doping. Journal of Physics Condensed Matter, 2021, 33, 314003.	1.8	10
104	Magnetic exchange interactions in bilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Cr</mml:mi><mml:msub><mml:mi>X</mml:mi></mml:msub><mml:mr assessment of the <mml:math xmlns:mml="http://www.w3.. Physical Review B, 2021, 103, .	3.2	10
105	Surface reconstructions and atomic ordering inInxGa1â^'xAs(001)films: A density-functional theory study. Physical Review B, 2006, 74, .	3.2	9
106	Surface morphology of MnSi thin films grown on Si(111). Surface Science, 2013, 617, 106-112.	1.9	9
107	Molybdenum Disulfide Nanoflakes Grown by Chemical Vapor Deposition on Graphite: Nucleation, Orientation, and Charge Transfer. Journal of Physical Chemistry C, 2020, 124, 2689-2697.	3.1	9
108	Detection of adsorbed transition-metal porphyrins by spin-dependent conductance of graphene nanoribbon. RSC Advances, 2017, 7, 29112-29121.	3.6	8

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109	Spin and orbital magnetism in orderedFe3Â±Î´Si1â^'Î´binary Heusler structures: Theory versus experiment. Physical Review B, 2008, 77, .	3.2	7
110	Linking density functional and density-matrix theory: Picosecond electron relaxation at the Si(100) surface. Physical Review B, 2008, 77, .	3.2	7
111	Modeling of minibands and electronic transport in one-dimensional stacks of InAs/GaAs quantum dots. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 906-910.	2.7	7
112	Theoretical prediction of improved figure-of-merit in Si/Ge quantum dot superlattices. New Journal of Physics, 2013, 15, 125010.	2.9	7
113	Interplay of hydrogen treatment and nitrogen doping in ZnO nanoparticles: a first-principles study. Nanotechnology, 2014, 25, 145204.	2.6	7
114	Reaction Dynamics of H2/Si: A 5-D Model. Springer Series in Solid-state Sciences, 1996, , 3-25.	0.3	7
115	Diffusion pathways of hydrogen across the steps of a vicinal Si(001) surface. Physical Review B, 2007, 75, .	3.2	6
116	Thermodynamics and Kinetics of Quantum Dot Growth. Nanoscience and Technology, 2008, , 1-39.	1.5	6
117	Theoretical investigation of the influence of isotope mass on chemicurrents during adsorption of H on K(110). Surface Science, 2010, 604, 1452-1458.	1.9	6
118	Atomistic calculation of the thermoelectric properties of Si nanowires. Physical Review B, 2014, 90, .	3.2	6
119	Thermoelectric properties of Ge/Si heterostructures: A combined theoretical and experimental study. Physica Status Solidi (A) Applications and Materials Science, 2016, 213, 524-532.	1.8	6
120	Coupling of quantum well states and phonons in thin multilayer Pb films on Si(111). Physical Review B, 2017, 96, .	3.2	6
121	Adsorption and dissociation of iron phthalocyanine on H/Si(111): Impact of van der Waals interactions and perspectives for subsurface doping. Physical Review B, 2019, 99, .	3.2	6
122	Isotopic effect on the vibrational lifetime of the carbon-deuterium stretch excitation on graphene. Journal of Chemical Physics, 2011, 135, 114506.	3.0	5
123	Large morphological sensitivity of the magneto-thermopower in Co/Cu multilayered systems. New Journal of Physics, 2015, 17, 033036.	2.9	5
124	Towards a standardized setup for surface energy calculations. Physical Review B, 2017, 95, .	3.2	5
125	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="italic">Ab</mml:mi><mml:mi mathvariant="italic">initio</mml:mi></mml:mrow></mml:math> simulation of the structure and transport properties of zirconium and ferromagnetic cobalt contacts on the two-dimensional semiconductor <mml:math	3.2	5
126	Electronic correlation, magnetic structure, and magnetotransport in few-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Cr</mml:mi><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2020, 4, .	2.4	5

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127	Theory of shape evolution of InAs quantum dots on In0.5Ga0.5As/InP(001) substrate. New Journal of Physics, 2009, 11, 073018.	2.9	4
128	Atomic-scale detection of magnetic impurity interactions in bulk semiconductors. Physical Review B, 2015, 92, .	3.2	4
129	Unoccupied electronic structure and momentum-dependent scattering dynamics in Pb/Si(557) nanowire arrays. Physical Review B, 2015, 92, .	3.2	4
130	Surface vibrations in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">T</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Pb phases on Si(111). Physical Review B, 2018, 98, .	3.2	4
131	Relaxation of electrons in quantum-confined states in Pb/Si(111) thin films from master equation with first-principles-derived rates. New Journal of Physics, 2019, 21, 123023.	2.9	4
132	Surface structural phase transition induced by the formation of metalâ€“organic networks on the Si(111)–In surface. Nanoscale, 2019, 11, 21790-21798.	5.6	4
133	A fresh look at the structure of aromatic thiols on Au surfaces from theory and experiment. Journal of Chemical Physics, 2021, 155, 044707.	3.0	4
134	STABILITY OF ADSORBED HYDROGEN ON Si(100) UNDER CHANGES OF THE SURFACE POTENTIAL. Surface Review and Letters, 1996, 03, 1227-1233.	1.1	3
135	Thermoelectric Properties of Half-Heusler Heterostructures from Ab Initio Calculations. Journal of Electronic Materials, 2016, 45, 1762-1766.	2.2	3
136	Boltzmann relaxation dynamics of strongly interacting spinless fermions on a lattice. Physical Review B, 2019, 100, .	3.2	3
137	Models for Hydrogen Extraction from the Passivated Si(100) Surface Induced by the Scanning Tunneling Microscope. Physica Status Solidi A, 1997, 159, 91-104.	1.7	2
138	Structure of GaAs(001)-c(4Ã—4): Comparison of X-ray diffraction and first-principles calculation. Surface Science, 2006, 600, 4099-4102.	1.9	2
139	Comment on â€œAngular distributions of H-induced HD and D2 desorptions from the Si(100) surfacesâ€•[J. Chem. Phys. 124, 054715 (2006)]. Journal of Chemical Physics, 2008, 128, 017101.	3.0	2
140	Ferromagnetic Heusler Alloy Thin Films: Electronic Properties and Magnetic Moment Formation. Springer Tracts in Modern Physics, 2013, , 119-162.	0.1	2
141	Single-atom vacancy in monolayer phosphorene: A comprehensive study of stability and magnetism under applied strain. Journal of Magnetism and Magnetic Materials, 2018, 465, 546-553.	2.3	2
142	Phonon-induced electronic relaxation in a strongly correlated system: The Sn/Si(111) <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:msqrt><mml:mn>3</mml:mn></mml:msqrt><mml:mo>×</mml:mo><mml:msqrt><mml:mn>3</mml:mn></mml:msqrt><mml:mo>)</mml:mo><mml:mi>R</mml:mi><mml:mn>30</mml:mn></mml:mrow></mml:math>° adlayer revisited. Physical Review B, 2019, 100, .	3.2	2
143	Gold-induced surface reconstruction on GaAs(111)Bsurface. Molecular Simulation, 2009, 35, 258-261.	2.0	1
144	Interface defects and impurities at the growth zone of Auâ€catalyzed GaAs nanowire from first principles. Physica Status Solidi - Rapid Research Letters, 2013, 7, 882-885.	2.4	1

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145	First-Principles Study of InAs/GaAs(001) Heteroepitaxy. , 2005, , 27-42.		1
146	Ab Initio Thermodynamics and Statistical Mechanics of Diffusion, Growth, and Self- Assembly of Quantum Dots. , 2002, , 355-369.		1
147	Atomistic Simulations of Processes at Surfaces. Springer Series in Materials Science, 2004, , 39-72.	0.6	0
148	Atomic processes in molecular beam epitaxy on strained InAs(137): A density-functional theory study. Physical Review B, 2009, 80, .	3.2	0
149	Optimized growth procedure for self-organized InAs quantum dots. Springer Proceedings in Physics, 2001, , 387-388.	0.2	0
150	Toward Predictive Growth Simulations: MBE on GaAs(001). Springer Proceedings in Physics, 2001, , 339-340.	0.2	0