Peter Kratzer

List of Publications by Year
in descending order

150 papers	5,286 citations	76031 42 h-index	111975 67 g-index
152 all docs	152 docs citations	152 times ranked	4927 citing authors

#	Article	IF	Citations
1	First-principles computational exploration of ferromagnetism in monolayer GaS via substitutional doping. Journal of Physics Condensed Matter, 2021, 33, 314003.	0.7	10
2	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:mr assessment of the <mml:math xmlns:mml="http://www.w3.. Physical Review B, 2021, 103, .	1.1	10
3	A fresh look at the structure of aromatic thiols on Au surfaces from theory and experiment. Journal of Chemical Physics, 2021, 155, 044707.	1.2	4
4	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.	1.2	14
5	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.	1.5	11
6	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.	1.5	26
7	Molybdenum Disulfide Nanoflakes Grown by Chemical Vapor Deposition on Graphite: Nucleation, Orientation, and Charge Transfer. Journal of Physical Chemistry C, 2020, 124, 2689-2697.	1.5	9
8	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, .	0.9	5
9	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.	1.5	20
10	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: adlayer revisited. Physical Review B, 2019, 100, .	1.1	2
11	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, .	1.1	6
12	The Basics of Electronic Structure Theory for Periodic Systems. Frontiers in Chemistry, 2019, 7, 106.	1.8	57
13	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.	1.2	4
14	Surface structural phase transition induced by the formation of metalâ€“organic networks on the Si(111)–In surface. Nanoscale, 2019, 11, 21790-21798.	2.8	4
15	Boltzmann relaxation dynamics of strongly interacting spinless fermions on a lattice. Physical Review B, 2019, 100, .	1.1	3
16	<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 xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="n	1.1	5
17	Spin caloric transport from density-functional theory. Journal Physics D: Applied Physics, 2019, 52, 073001.	1.3	13
18	Band structure and thermoelectric properties of half-Heusler semiconductors from many-body perturbation theory. Physical Review B, 2018, 97, .	1.1	43

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19	Enhanced electronic and magnetic properties by functionalization of monolayer GaS via substitutional doping and adsorption. Journal of Physics Condensed Matter, 2018, 30, 195805.	0.7	11
20	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, .	1.1	4
21	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.	1.0	2
22	Commensurate versus incommensurate heterostructures of group-III monochalcogenides. Physical Review Materials, 2018, 2, .	0.9	19
23	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.	1.2	11
24	Crystal Structure Induced Preferential Surface Alloying of Sb on Wurtzite/Zinc Blende GaAs Nanowires. Nano Letters, 2017, 17, 3634-3640.	4.5	14
25	Coupling of quantum well states and phonons in thin multilayer Pb films on Si(111). Physical Review B, 2017, 96, .	1.1	6
26	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: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>(</mml:mo><mml:mrow><mml:mi>Z</mml:mi><mml:mo>=</mml:mo> full Heusler alloys: Formation and. Physical Review B, 2017, 96, .	1.1	24
27	Towards a standardized setup for surface energy calculations. Physical Review B, 2017, 95, .	1.1	5
28	Magnetic monolayer Li 2 N: Density Functional Theory calculations. Europhysics Letters, 2017, 119, 57002.	0.7	13
29	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— -In surface. Physical Review B, 2017, 96, .	1.1	15
30	Detection of adsorbed transition-metal porphyrins by spin-dependent conductance of graphene nanoribbon. RSC Advances, 2017, 7, 29112-29121.	1.7	8
31	Ternary semiconductors NiZrSn and CoZrBi with half-Heusler structure: A first-principles study. Physical Review B, 2016, 94, .	1.1	32
32	Thermoelectric properties of Ge/Si heterostructures: A combined theoretical and experimental study. Physica Status Solidi (A) Applications and Materials Science, 2016, 213, 524-532.	0.8	6
33	Thermoelectric Properties of Half-Heusler Heterostructures from Ab Initio Calculations. Journal of Electronic Materials, 2016, 45, 1762-1766.	1.0	3
34	Atomic-scale detection of magnetic impurity interactions in bulk semiconductors. Physical Review B, 2015, 92, .	1.1	4
35	Unoccupied electronic structure and momentum-dependent scattering dynamics in Pb/Si(557) nanowire arrays. Physical Review B, 2015, 92, .	1.1	4
36	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:msub></mml: tunnel junctions. Physical Review B, 2015, 92, .	1.1	29

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37	Reduced thermal conductivity of TiNiSn/HfNiSn superlattices. Physical Review B, 2015, 92, .	1.1	33
38	Large morphological sensitivity of the magneto-thermopower in Co/Cu multilayered systems. New Journal of Physics, 2015, 17, 033036.	1.2	5
39	Electronic and Structural Differences between Wurtzite and Zinc Blende InAs Nanowire Surfaces: Experiment and Theory. ACS Nano, 2014, 8, 12346-12355.	7.3	78
40	Atomistic calculation of the thermoelectric properties of Si nanowires. Physical Review B, 2014, 90, .	1.1	6
41	Interplay of hydrogen treatment and nitrogen doping in ZnO nanoparticles: a first-principles study. Nanotechnology, 2014, 25, 145204.	1.3	7
42	First-principles study of spin-dependent thermoelectric properties of half-metallic Heusler thin films between platinum leads. Physical Review B, 2014, 89, .	1.1	56
43	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:m xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>Al/Co</mml:mtext><mml:mn>2</mml:mn></mml:m Physical Review B, 2014, 89, .	1.1	19
44	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.	1.2	1
45	Large Seebeck magnetic anisotropy in thin Co films embedded in Cu determined byab initioinvestigations. Physical Review B, 2013, 88, .	1.1	12
46	Ferromagnetic Heusler Alloy Thin Films: Electronic Properties and Magnetic Moment Formation. Springer Tracts in Modern Physics, 2013, , 119-162.	0.1	2
47	Surface morphology of MnSi thin films grown on Si(111). Surface Science, 2013, 617, 106-112.	0.8	9
48	Comparison of density functionals for nitrogen impurities in ZnO. Journal of Chemical Physics, 2013, 138, 234702.	1.2	13
49	Theoretical prediction of improved figure-of-merit in Si/Ge quantum dot superlattices. New Journal of Physics, 2013, 15, 125010.	1.2	7
50	Strain stabilization and thickness dependence of magnetism in epitaxial transition metal monosilicide thin films on Si(111). Physical Review B, 2013, 88, .	1.1	16
51	Atomistic modeling of the Au dropletâ€“GaAs interface for size-selective nanowire growth. Physical Review B, 2013, 88, .	1.1	21
52	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, .	1.1	15
53	As vacancies, Ga antisites, and Au impurities in zinc blende and wurtzite GaAs nanowire segments from first principles. Physical Review B, 2013, 87, .	1.1	27
54	Growth mode and atomic structure of MnSi thin films on Si(111). Physical Review B, 2012, 86, .	1.1	33

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55	Anisotropic ferromagnetism in carbon-doped zinc oxide from first-principles studies. Physical Review B, 2012, 86, .	1.1	31
56	Role of sidewall diffusion in GaAs nanowire growth: A first-principles study. Physical Review B, 2012, 86, .	1.1	25
57	Catalytic Role of Gold Nanoparticle in GaAs Nanowire Growth: A Density Functional Theory Study. Nano Letters, 2012, 12, 943-948.	4.5	30
58	Density functional study of carbon doping in ZnO. Semiconductor Science and Technology, 2011, 26, 014038.	1.0	24
59	Analytic many-body potential for GaAs(001) homoepitaxy: Bulk and surface properties. Physical Review B, 2011, 83, .	1.1	18
60	Calculation of the diameter-dependent polytypism in GaAs nanowires from an atomic motif expansion of the formation energy. Physical Review B, 2011, 84, .	1.1	53
61	Isotopic effect on the vibrational lifetime of the carbon-deuterium stretch excitation on graphene. Journal of Chemical Physics, 2011, 135, 114506.	1.2	5
62	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.	1.3	7
63	Theoretical investigation of the influence of isotope mass on chemicurrents during adsorption of H on K(110). Surface Science, 2010, 604, 1452-1458.	0.8	6
64	Hydrogen vibrational modes on graphene and relaxation of the Câ€“H stretch excitation from first-principles calculations. Journal of Chemical Physics, 2010, 133, 054505.	1.2	40
65	Magnetism in C- or N-doped MgO and ZnO: A Density-Functional Study of Impurity Pairs. Physical Review Letters, 2010, 105, 267203.	2.9	111
66	Thermoelectric transport in periodic one-dimensional stacks of InAs/GaAs quantum dots. Physical Review B, 2010, 82, .	1.1	26
67	Electronic excitations in magnesium epitaxy: Experiment and theory. Physical Review B, 2010, 82, .	1.1	13
68	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><mml:mn wetting layers on GaAs(001). Physical Review B, 2009, 79, .	1.1	29
69	Electron-hole spectra created by adsorption on metals from density functional theory. Physical Review B, 2009, 79, .	1.1	31
70	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.	1.1	28
71	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 ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 92 Td (stretchy="fals A Density Functional Theory Study. Physical Review Letters, 2009, 103, 046803.	2.9	37
72	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 A combined density functional theory and cluster expansion s. Physical Review B, 2009, 79, .	1.1	62

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73	Atomic processes in molecular beam epitaxy on strained InAs(137): A density-functional theory study. Physical Review B, 2009, 80, .	1.1	0
74	Isotope effects in the vibrational lifetime of hydrogen on germanium(100): Theory and experiment. Journal of Chemical Physics, 2009, 131, 124502.	1.2	13
75	Theory of shape evolution of InAs quantum dots on In0.5Ga0.5As/InP(001) substrate. New Journal of Physics, 2009, 11, 073018.	1.2	4
76	Gold-induced surface reconstruction on GaAs(111)Bsurface. Molecular Simulation, 2009, 35, 258-261.	0.9	1
77	Searching for Si-based spintronics by first principles calculations. New Journal of Physics, 2009, 11, 125009.	1.2	14
78	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.	0.7	16
79	Ordering of the Nanoscale Step Morphology As a Mechanism for Droplet Self-Propulsion. Nano Letters, 2009, 9, 2710-2714.	4.5	66
80	Thermodynamics and Kinetics of Quantum Dot Growth. Nanoscience and Technology, 2008, , 1-39.	1.5	6
81	Adsorption of indium on an InAs wetting layer deposited on the GaAs(001) surface. Physical Review B, 2008, 77, .	1.1	14
82	Exchange interactions and critical temperature of bulk and thin films of MnSi: A density functional theory study. Physical Review B, 2008, 78, .	1.1	46
83	Density-functional theory study of vibrational relaxation of CO stretching excitation on Si(100). Journal of Chemical Physics, 2008, 129, 174702.	1.2	27
84	Direct Atomic Scale Imaging of IIIâ^'V Nanowire Surfaces. Nano Letters, 2008, 8, 3978-3982.	4.5	59
85	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.	1.2	2
86	Spin and orbital magnetism in orderedFe3Â±Î´Si1â^'Î´binary Heusler structures: Theory versus experiment. Physical Review B, 2008, 77, .	1.1	7
87	Analytic many-body potential for InAs/GaAs surfaces and nanostructures: Formation energy of InAs quantum dots. Physical Review B, 2008, 77, .	1.1	57
88	Linking density functional and density-matrix theory: Picosecond electron relaxation at the Si(100) surface. Physical Review B, 2008, 77, .	1.1	7
89	Transition-metal silicides as materials for magnet-semiconductor heterostructures. Journal of Applied Physics, 2007, 101, 081725.	1.1	14
90	Electronic structure changes ofSi(001)â^'(2Ã—1)from subsurface Mn observed by STM. Physical Review B, 2007, 75, .	1.1	28

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91	Density-Functional Theory Study of Half-Metallic Heterostructures: Interstitial Mn in Si. Physical Review Letters, 2007, 98, 117202.	2.9	71
92	Diffusion pathways of hydrogen across the steps of a vicinal Si(001) surface. Physical Review B, 2007, 75, .	1.1	6
93	Density-functional study of Mn monosilicide on the Si(111) surface: Film formation versus island nucleation. Physical Review B, 2007, 76, .	1.1	30
94	Elastic response of cubic crystals to biaxial strain: Analytic results and comparison to density functional theory for InAs. Physical Review B, 2007, 75, .	1.1	35
95	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.	1.1	14
96	Shape transition during epitaxial growth ofInAsquantum dots onGaAs(001): Theory and experiment. Physical Review B, 2006, 73, .	1.1	80
97	Epitaxy of Mn on Si(001): Adsorption, surface diffusion, and magnetic properties studied by density-functional theory. Physical Review B, 2006, 74, .	1.1	54
98	Structure of GaAs(001)-c(4Ã—4): Comparison of X-ray diffraction and first-principles calculation. Surface Science, 2006, 600, 4099-4102.	0.8	2
99	Control of fine-structure splitting and excitonic binding energies in selected individual InAsâ•GaAs quantum dots. Applied Physics Letters, 2006, 89, 263109.	1.5	60
100	Surface reconstructions and atomic ordering inInxGa1â’xAs(001)films: A density-functional theory study. Physical Review B, 2006, 74, .	1.1	9
101	Au wetting and nanoparticle stability on GaAs(111)B. Applied Physics Letters, 2006, 89, 251912.	1.5	20
102	First-principles study of thin magnetic transition-metal silicide films on Si(001). Physical Review B, 2005, 72, .	1.1	45
103	Preserving the Half-Metallicity at the Heusler AlloyCo2MnSi(001)Surface: A Density Functional Theory Study. Physical Review Letters, 2005, 94, 096402.	2.9	167
104	First-Principles Study of InAs/GaAs(001) Heteroepitaxy. , 2005, , 27-42.		1
105	Atomic Structure of theGaAs(001)â’c(4Ã—4)Surface: First-Principles Evidence For Diversity of Heterodimer Motifs. Physical Review Letters, 2004, 93, 146102.	2.9	39
106	Structure and morphology of the As-rich and the stoichiometric GaAs(114)A surface. Journal of Applied Physics, 2004, 95, 7645-7654.	1.1	11
107	Anisotropic diffusion of In adatoms on pseudomorphicInxGa1â’xAsfilms: First-principles total energy calculations. Physical Review B, 2004, 69, .	1.1	52
108	Atomistic Simulations of Processes at Surfaces. Springer Series in Materials Science, 2004, , 39-72.	0.4	0

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109	First-Principles Study of Ferromagnetism in Epitaxial Si-Mn Thin Films on Si(001). Physical Review Letters, 2004, 92, 237202.	2.9	66
110	Understanding the growth mechanisms of GaAs and InGaAs thin films by employing first-principles calculations. Applied Surface Science, 2003, 216, 436-446.	3.1	77
111	Tight-binding study of the influence of the strain on the electronic properties of InAs/GaAs quantum dots. Physical Review B, 2003, 68, .	1.1	81
112	InAs quantum dots grown on theGaAs(113)AandGaAs(1Â¯1Â¯3Â¯)Bsurfaces: A comparative STM study. Physical Review B, 2003, 68, .	1.1	30
113	Surface structure of GaAs(2 5 11). Physical Review B, 2002, 65, .	1.1	24
114	Reaction-Limited Island Nucleation in Molecular Beam Epitaxy of Compound Semiconductors. Physical Review Letters, 2002, 88, 036102.	2.9	88
115	Quantum Monte Carlo Calculations ofH2Dissociation on Si(001). Physical Review Letters, 2002, 89, 166102.	2.9	83
116	First-principles studies of kinetics in epitaxial growth of III-V semiconductors. Applied Physics A: Materials Science and Processing, 2002, 75, 79-88.	1.1	86
117	Ab Initio Thermodynamics and Statistical Mechanics of Diffusion, Growth, and Self- Assembly of Quantum Dots. , 2002, , 355-369.		1
118	Effect of strain on surface diffusion in semiconductor heteroepitaxy. Physical Review B, 2001, 64, .	1.1	92
119	Surface knowledge: toward a predictive theory of materials. Computing in Science and Engineering, 2001, 3, 16-25.	1.2	21
120	Island dissolution during capping layer growth interruption. Applied Physics A: Materials Science and Processing, 2001, 73, 161-165.	1.1	27
121	GaAs(2511): A New Stable Surface within the Stereographic Triangle. Physical Review Letters, 2001, 86, 3815-3818.	2.9	49
122	Atomic Structure of the Stoichiometric GaAs(114) Surface. Physical Review Letters, 2001, 86, 115-118.	2.9	28
123	Role of Electronic Correlation in the Si(100) Reconstruction: A Quantum Monte Carlo Study. Physical Review Letters, 2001, 87, 016105.	2.9	146
124	Probing Interface Electronic Structure with Overlayer Quantum-Well Resonances:Al/Si(111). Physical Review Letters, 2001, 87, 156801.	2.9	95
125	Optimized growth procedure for self-organized InAs quantum dots. Springer Proceedings in Physics, 2001, , 387-388.	0.1	0
126	Toward Predictive Growth Simulations: MBE on GaAs(001). Springer Proceedings in Physics, 2001, , 339-340.	0.1	0

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127	Size, shape, and stability of InAs quantum dots on the GaAs(001) substrate. Physical Review B, 2000, 62, 1897-1904.	1.1	96
128	Energetics of InAs Thin Films and Islands on the GaAs(001) Substrate. Japanese Journal of Applied Physics, 2000, 39, 4298-4301.	0.8	17
129	Formation and Stability of Self-Assembled Coherent Islands in Highly Mismatched Heteroepitaxy. Physical Review Letters, 1999, 82, 4042-4045.	2.9	147
130	Effect of the cluster size in modeling the H2 desorption and dissociative adsorption on Si(001). Journal of Chemical Physics, 1999, 110, 3986-3994.	1.2	162
131	Model for nucleation in GaAs homoepitaxy derived from first principles. Physical Review B, 1999, 59, 15246-15252.	1.1	47
132	Arsenic Dimer Dynamics during MBE Growth: Theoretical Evidence for a Novel Chemisorption State ofAs2Molecules on GaAs Surfaces. Physical Review Letters, 1999, 82, 4886-4889.	2.9	83
133	Density-functional study of hydrogen chemisorption on vicinal Si(001) surfaces. Physical Review B, 1999, 59, 2790-2800.	1.1	34
134	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.	2.9	159
135	The dynamics of the H + D/Si(001) reaction: a trajectory study based on ab initio potentials. Chemical Physics Letters, 1998, 288, 396-402.	1.2	26
136	Density-functional theory studies on microscopic processes of gaas growth. Progress in Surface Science, 1998, 59, 135-147.	3.8	22
137	Highly Site-SpecificH2Adsorption on VicinalSi(001)Surfaces. Physical Review Letters, 1998, 81, 5596-5599.	2.9	100
138	Reaction dynamics of atomic hydrogen with the hydrogenated Si(001) (2Ã—1) surface. Journal of Chemical Physics, 1997, 106, 6752-6763.	1.2	87
139	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
140	Ab initio quantum dynamics of adsorption/desorption on a 3-D potential. Surface Science, 1996, 345, 125-137.	0.8	31
141	Geometric and electronic factors determining the differences in reactivity of H2 on Cu(100) and Cu(111). Surface Science, 1996, 359, 45-53.	0.8	100
142	Designing surface alloys with specific active sites. Catalysis Letters, 1996, 40, 131-135.	1.4	77
143	Reaction dynamics of molecular hydrogen on silicon surfaces. Physical Review B, 1996, 54, 5978-5991.	1.1	75
144	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.	1.2	30

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145	A theoretical study of CH4 dissociation on pure and goldâ€alloyed Ni(111) surfaces. Journal of Chemical Physics, 1996, 105, 5595-5604.	1.2	262
146	STABILITY OF ADSORBED HYDROGEN ON Si(100) UNDER CHANGES OF THE SURFACE POTENTIAL. Surface Review and Letters, 1996, 03, 1227-1233.	0.5	3
147	Reaction Dynamics of H2/Si: A 5-D Model. Springer Series in Solid-state Sciences, 1996, , 3-25.	0.3	7
148	Direct pathway for sticking/desorption ofH2on Si(100). Physical Review B, 1995, 51, 13432-13440.	1.1	84
149	The coupling between adsorption dynamics and the surface structure: H2 on Si(100). Chemical Physics Letters, 1994, 229, 645-649.	1.2	65
150	Highly excited molecules from Eley-Rideal reactions. Surface Science, 1991, 254, 275-280.	0.8	93