Matthias Scheffler

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3008484/publications.pdf

Version: 2024-02-01

386	56,980	643 123	1158 229
papers	citations	h-index	g-index

398	398	398	33956
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Learning Design Rules for Selective Oxidation Catalysts from High-Throughput Experimentation and Artificial Intelligence. ACS Catalysis, 2022, 12, 2223-2232.	11.2	22
2	Artificial-intelligence-driven discovery of catalyst genes with application to CO2 activation on semiconductor oxides. Nature Communications, 2022, 13, 419.	12.8	45
3	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	2.8	69
4	SISSO++: A C++ Implementation of the Sure-Independence Screening and Sparsifying Operator Approach. Journal of Open Source Software, 2022, 7, 3960.	4.6	8
5	Numerical quality control for DFT-based materials databases. Npj Computational Materials, 2022, 8, .	8.7	6
6	FAIR data enabling new horizons for materials research. Nature, 2022, 604, 635-642.	27.8	81
7	<i>AbÂInitio</i> Approach for Thermodynamic Surface Phases with Full Consideration of Anharmonic Effects: The Example of Hydrogen at Si(100). Physical Review Letters, 2022, 128, .	7.8	1
8	Interface to high-performance periodic coupled-cluster theory calculations with atom-centered, localized basis functions. Journal of Open Source Software, 2022, 7, 4040.	4.6	0
9	All-electron periodic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mm implementation with numerical atomic orbital basis functions: Algorithm and benchmarks. Physical Review Materials, 2021, 5, .	2.4	25
10	OPTIMADE, an API for exchanging materials data. Scientific Data, 2021, 8, 217.	5.3	49
11	Materials genes of heterogeneous catalysis from clean experiments and artificial intelligence. MRS Bulletin, 2021, 46, 1016-1026.	3.5	26
12	GIMS: Graphical Interface for Materials Simulations. Journal of Open Source Software, 2021, 6, 2767.	4.6	1
13	Roadmap on organicâ€“inorganic hybrid perovskite semiconductors and devices. APL Materials, 2021, 9, .	5.1	102
14	Towards Experimental Handbooks in Catalysis. Topics in Catalysis, 2020, 63, 1683-1699.	2.8	28
15	Fully anharmonic nonperturbative theory of vibronically renormalized electronic band structures. Physical Review B, 2020, 102, .	3.2	30
16	Identifying domains of applicability of machine learning models for materials science. Nature Communications, 2020, 11, 4428.	12.8	66
17	Big Data-Driven Materials Science and Its FAIR Data Infrastructure. , 2020, , 49-73.		18
18	Pentacene and tetracene molecules and films on H/Si(111): level alignment from hybrid density functional theory. Electronic Structure, 2020, 2, 035002.	2.8	15

#	Article	IF	Citations
19	Artificial intelligence for high-throughput discovery of topological insulators: The example of alloyed tetradymites. Physical Review Materials, 2020, 4, .	2.4	25
20	Anharmonicity measure for materials. Physical Review Materials, 2020, 4, .	2.4	45
21	FHI-vibes: Ab Initio Vibrational Simulations. Journal of Open Source Software, 2020, 5, 2671.	4.6	15
22	Benefits from using mixed precision computations in the ELPA-AEO and ESSEX-II eigensolver projects. Japan Journal of Industrial and Applied Mathematics, 2019, 36, 699-717.	0.9	10
23	Massive-Parallel Implementation of the Resolution-of-Identity Coupled-Cluster Approaches in the Numeric Atom-Centered Orbital Framework for Molecular Systems. Journal of Chemical Theory and Computation, 2019, 15, 4721-4734.	5.3	22
24	Determining surface phase diagrams including anharmonic effects. Physical Review B, 2019, 100, .	3.2	9
25	Simultaneous learning of several materials properties from incomplete databases with multi-task SISSO. JPhys Materials, 2019, 2, 024002.	4.2	97
26	Modulation of the Work Function by the Atomic Structure of Strong Organic Electron Acceptors on Hâ€ši(111). Advanced Electronic Materials, 2019, 5, 1800891.	5.1	30
27	Main-group test set for materials science and engineering with user-friendly graphical tools for error analysis: systematic benchmark of the numerical and intrinsic errors in state-of-the-art electronic-structure approximations. New Journal of Physics, 2019, 21, 013025.	2.9	15
28	The NOMAD laboratory: from data sharing to artificial intelligence. JPhys Materials, 2019, 2, 036001.	4.2	171
29	New tolerance factor to predict the stability of perovskite oxides and halides. Science Advances, 2019, 5, eaav0693.	10.3	778
30	Beyond Scaling Relations for the Description of Catalytic Materials. ACS Catalysis, 2019, 9, 2752-2759.	11.2	157
31	Parametrically constrained geometry relaxations for high-throughput materials science. Npj Computational Materials, 2019, 5, .	8.7	13
32	Crowd-sourcing materials-science challenges with the NOMAD 2018 Kaggle competition. Npj Computational Materials, 2019, 5, .	8.7	39
33	Compact representation of one-particle wavefunctions and scalar fields obtained from electronic-structure calculations. Computer Physics Communications, 2019, 237, 42-46.	7.5	0
34	Big Data-Driven Materials Science and Its FAIR Data Infrastructure. , 2019, , 1-25.		5
35	Two-to-three dimensional transition in neutral gold clusters: The crucial role of van der Waals interactions and temperature. Physical Review Materials, 2019, 3, .	2.4	40
36	Electron-phonon coupling in d -electron solids: A temperature-dependent study of rutile TiO2 by first-principles theory and two-photon photoemission. Physical Review Research, 2019, 1, .	3.6	6

#	Article	IF	Citations
37	First-principles supercell calculations of small polarons with proper account for long-range polarization effects. New Journal of Physics, 2018, 20, 033023.	2.9	43
38	Local Atomic Arrangements and Band Structure of Boron Carbide. Angewandte Chemie - International Edition, 2018, 57, 6130-6135.	13.8	39
39	NOMAD: The FAIR concept for big data-driven materials science. MRS Bulletin, 2018, 43, 676-682.	3.5	288
40	All-electron, real-space perturbation theory for homogeneous electric fields: theory, implementation, and application within DFT. New Journal of Physics, 2018, 20, 073040.	2.9	36
41	Performance of various density-functional approximations for cohesive properties of 64 bulk solids. New Journal of Physics, 2018, 20, 063020.	2.9	185
42	Insightful classification of crystal structures using deep learning. Nature Communications, 2018, 9, 2775.	12.8	237
43	SISSO: A compressed-sensing method for identifying the best low-dimensional descriptor in an immensity of offered candidates. Physical Review Materials, 2018, 2, .	2.4	349
44	Lattice dynamics calculations based on density-functional perturbation theory in real space. Computer Physics Communications, 2017, 215, 26-46.	7.5	51
45	Understanding band gaps of solids in generalized Kohnâ€“Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	7.1	423
46	Learning physical descriptors for materials science by compressed sensing. New Journal of Physics, 2017, 19, 023017.	2.9	100
47	Li/MgO Catalysts Doped with Alioâ€valent Ions. Part II: Local Topology Unraveled by EPR/NMR and DFT Modeling. ChemCatChem, 2017, 9, 3597-3610.	3.7	11
48	Open data settled in materials theory. Nature, 2017, 548, 523-523.	27.8	6
49	Uncovering structure-property relationships of materials by subgroup discovery. New Journal of Physics, 2017, 19, 013031.	2.9	77
50	Formation of Vacancies in Si- and Ge-based Clathrates: Role of Electron Localization and Symmetry Breaking. Physical Review Letters, 2017, 118, 236401.	7.8	20
51	Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. Npj Computational Materials, 2017, 3, .	8.7	79
52	AbÂInitio Green-Kubo Approach for the Thermal Conductivity of Solids. Physical Review Letters, 2017, 118, 175901.	7.8	83
53	Obituary for Walter Kohn (1923â€“2016). Computation, 2016, 4, 40.	2.0	3
54	Wave-function inspired density functional applied to the H₂/${{m{H}}}_{2}^{+}$ challenge. New Journal of Physics, 2016, 18, 073026.	2.9	12

#	Article	IF	Citations
55	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. Physical Review Letters, 2016, 117, 133002.	7.8	24
56	Density functional theory study of theÎ±â˜Î³phase transition in cerium: Role of electron correlation andf-orbital localization. Physical Review B, 2016, 93, .	3.2	23
57	Enforcing the linear behavior of the total energy with hybrid functionals: Implications for charge transfer, interaction energies, and the random-phase approximation. Physical Review B, 2016, 94, .	3.2	52
58	Self-consistent Green's function embedding for advanced electronic structure methods based on a dynamical mean-field concept. Physical Review B, 2016, 93, .	3.2	34
59	Walter Kohn (1923â€“2016). Nature Materials, 2016, 15, 704-704.	27.5	0
60	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
61	Accurate localized resolution of identity approach for linear-scaling hybrid density functionals and for many-body perturbation theory. New Journal of Physics, 2015, 17, 093020.	2.9	97
62	Why graphene growth is very different on the C face than on the Si face of SiC: Insights from surface equilibria and the<mml:math		

#	Article	IF	Citations
73	Evidence for photogenerated intermediate hole polarons in ZnO. Nature Communications, 2015, 6, 6901.	12.8	53
74	Native like helices in a specially designed Î² peptide in the gas phase. Physical Chemistry Chemical Physics, 2015, 17, 5376-5385.	2.8	14
75	GW100: Benchmarking G₀W₀ for Molecular Systems. Journal of Chemical Theory and Computation, 2015, 11, 5665-5687.	5.3	280
76	Exploring the conformational preferences of 20-residue peptides in isolation: Ac-Ala₁₉-Lys + H⁺vs. Ac-Lys-Ala₁₉ + H⁺ and the current reach of DFT. Physical Chemistry Chemical Physics, 2015, 17, 7373-7385.	2.8	48
77	Efficientab initioschemes for finding thermodynamically stable and metastable atomic structures: benchmark of cascade genetic algorithms. New Journal of Physics, 2014, 16, 123016.	2.9	37
78	How mono-valent cations bend peptide turns and a first-principles database of amino acids and dipeptides. , 2014, , .		0
79	Origins of optical absorption and emission lines in AlN. Applied Physics Letters, 2014, 105, .	3.3	127
80	Ferroelastic switching of doped zirconia: Modeling and understanding from first principles. Physical Review B, 2014, 90, .	3.2	28
81	Validation Challenge of Density-Functional Theory for Peptidesâ€"Example of Ac-Phe-Ala₅-LysH⁺. Journal of Physical Chemistry A, 2014, 118, 7349-7359.	2.5	43
82	First-principles description of charge transfer in donor-acceptor compounds from self-consistent many-body perturbation theory. Physical Review B, 2014, 90, .	3.2	44
83	Effects of strain on the band structure of group-III nitrides. Physical Review B, 2014, 90, .	3.2	100
84	Modeling Adsorption and Reactions of Organic Molecules at Metal Surfaces. Accounts of Chemical Research, 2014, 47, 3369-3377.	15.6	218
85	Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies. Journal of Chemical Theory and Computation, 2013, 9, 3404-3419.	5.3	499
86	Thermodynamic Equilibrium Conditions of Graphene Films on SiC. Physical Review Letters, 2013, 111, 065502.	7.8	34
87	How Cations Change Peptide Structure. Chemistry - A European Journal, 2013, 19, 11224-11234.	3.3	36
88	Stability and Metastability of Clusters in a Reactive Atmosphere: Theoretical Evidence for Unexpected Stoichiometries of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Mg</mml:mi><mml:mi>M</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math>. Physical Review Letters, 2013, 111, 135501.	7.8	72
89	How a Simple Sequence Change Induces Antipodal Folding Characteristics: Ac-Ala19-Lys + H+ Vs. Ac-Lys-Ala19 + H+. Biophysical Journal, 2013, 104, 55a.	0.5	0
90	Self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>: All-electron implementation with localized basis functions. Physical Review B, 2013, 88, .	3.2	135

#	Article	IF	Citations
91	Bond Breaking and Bond Formation: How Electron Correlation is Captured in Many-Body Perturbation Theory and Density-Functional Theory. Physical Review Letters, 2013, 110, 146403.	7.8	82
92	Controlling the work function of ZnO and the energy-level alignment at the interface to organic semiconductors with a molecular electron acceptor. Physical Review B, 2013, 87, .	3.2	109
93	FHI-gap: A code based on the all-electron augmented plane wave method. Computer Physics Communications, 2013, 184, 348-366.	7.5	56
94	Space-Charge Transfer in Hybrid Inorganic-Organic Systems. Physical Review Letters, 2013, 111, 226802.	7.8	68
95	Hybrid density functional theory meets quasiparticle calculations: A consistent electronic structure approach. Physical Review B, 2013, 88, .	3.2	115
96	Impact of Vibrational Entropy on the Stability of Unsolvated Peptide Helices with Increasing Length. Journal of Physical Chemistry B, 2013, 117, 5574-5584.	2.6	35
97	Oxidative Dehydrogenation of Methane by Isolated Vanadium Oxide Clusters Supported on Au (111) and Ag (111) Surfaces. Journal of Physical Chemistry C, 2013, 117, 18475-18483.	3.1	8
98	Structure and energetics of benzene adsorbed on transition-metal surfaces: density-functional theory with van der Waals interactions including collective substrate response. New Journal of Physics, 2013, 15, 053046.	2.9	143
99	Not so loosely bound rare gas atoms: finite-temperature vibrational fingerprints of neutral gold-cluster complexes. New Journal of Physics, 2013, 15, 083003.	2.9	56
100	Interface dipoles of organic molecules on Ag(111) in hybrid density-functional theory. New Journal of Physics, 2013, 15, 123028.	2.9	58
101	Concentration of Vacancies at Metal-Oxide Surfaces: Case Study of MgO(100). Physical Review Letters, 2013, 111, 045502.	7.8	104
102	Large work function reduction by adsorption of a molecule with a negative electron affinity: Pyridine on ZnO$(10ar{1}0)$(101Â¯). Journal of Chemical Physics, 2013, 139, 174701.	3.0	68
103	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. New Journal of Physics, 2013, 15, 123033.	2.9	81
104	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. Physical Review B, 2013, 88, .	3.2	113
105	On the accuracy of van der Waals inclusive density-functional theory exchange-correlation functionals for ice at ambient and high pressures. Journal of Chemical Physics, 2013, 139, 154702.	3.0	119
106	Assessment of correlation energies based on the random-phase approximation. New Journal of Physics, 2012, 14, 043002.	2.9	137
107	Impact of widely used approximations to theG₀W₀method: an all-electron perspective. New Journal of Physics, 2012, 14, 023006.	2.9	38
108	Benzene adsorbed on Si(001): The role of electron correlation and finite temperature. Physical Review B, 2012, 85, .	3.2	28

#	Article	IF	Citations
109	Accurate and Efficient Method for Many-Body van der Waals Interactions. Physical Review Letters, 2012, 108, 236402.	7.8	1,120
110	Density-Functional Theory for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>f</mml:mi></mml:math>-Electron Systems: The<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:mi>Î³</mml:mi></mml:math>Phase Transition in Cerium. Physical Review Letters, 2012, 109, 146402.	7.8	62
111	Random-phase approximation and its applications in computational chemistry and materials science. Journal of Materials Science, 2012, 47, 7447-7471.	3.7	479
112	Strain effects and band parameters in MgO, ZnO, and CdO. Applied Physics Letters, 2012, 101, .	3.3	67
113	Electronic properties of lanthanide oxides from the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>perspective. Physical Review B, 2012, 86, .	3.2	96
114	Role of nitrogen vacancies in the luminescence of Mg-doped GaN. Applied Physics Letters, 2012, 100, .	3.3	136
115	New Perspective on Formation Energies and Energy Levels of Point Defects in Nonmetals. Physical Review Letters, 2012, 108, 066404.	7.8	96
116	Toward Low-Temperature Dehydrogenation Catalysis: Isophorone Adsorbed on Pd(111). Journal of Physical Chemistry Letters, 2012, 3, 582-586.	4.6	33
117	Benchmark of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>methods for azabenzenes. Physical Review B, 2012, 86, .	3.2	154
118	Local Conformational Preferences of Peptides Near Attached Cations: Structure Determination by First-Principles Theory and IR-Spectroscopy. Biophysical Journal, 2012, 102, 46a.	0.5	0
119	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. Physical Review B, 2012, 86, .	3.2	243
120	Density-Functional Theory with Screened vanÂderÂWaals Interactions for the Modeling of Hybrid Inorganic-Organic Systems. Physical Review Letters, 2012, 108, 146103.	7.8	503
121	First-Principles Optical Spectra for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>F</mml:mi></mml:math>Centers in MgO. Physical Review Letters, 2012, 108, 126404.	7.8	157
122	Resolution-of-identity approach to Hartreeâ€“Fock, hybrid density functionals, RPA, MP2 andGWwith numeric atom-centered orbital basis functions. New Journal of Physics, 2012, 14, 053020.	2.9	549
123	Hydrogen Bonds and van der Waals Forces in Ice at Ambient and High Pressures. Physical Review Letters, 2011, 107, 185701.	7.8	193
124	Free gold clusters: beyond the static, monostructure description. Faraday Discussions, 2011, 152, 153.	3.2	39
125	Beyond the Random-Phase Approximation for the Electron Correlation Energy: The Importance of Single Excitations. Physical Review Letters, 2011, 106, 153003.	7.8	193
126	A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane. Catalysis Reviews - Science and Engineering, 2011, 53, 424-514.	12.9	205

#	Article	IF	Citations
127	van der Waals Interactions in Ionic and Semiconductor Solids. Physical Review Letters, 2011, 107, 245501.	7.8	143
128	Analytic many-body potential for GaAs(001) homoepitaxy: Bulk and surface properties. Physical Review B, 2011, 83, .	3.2	18
129	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3944-3951.	5.3	265
130	Activation Energies for Diffusion of Defects in Silicon: The Role of the Exchangeâ€Correlation Functional. Angewandte Chemie - International Edition, 2011, 50, 10221-10225.	13.8	31
131	CO Oxidation as a Prototypical Reaction for Heterogeneous Processes. Angewandte Chemie - International Edition, 2011, 50, 10064-10094.	13.8	639
132	Enhanced dipole moments in photo-excited TTFâ€“TCNQ dimers. New Journal of Physics, 2011, 13, 073039.	2.9	8
133	Unraveling the Stability of Polypeptide Helices: Critical Role of van der Waals Interactions. Physical Review Letters, 2011, 106, 118102.	7.8	97
134	Band parameters and strain effects in ZnO and group-III nitrides. Semiconductor Science and Technology, 2011, 26, 014037.	2.0	56
135	Electronic band structure of zirconia and hafnia polymorphs from the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>perspective. Physical Review B, 2010, 81, .	3.2	191
136	Alloy Catalyst in a Reactive Environment: The Example of Ag-Cu Particles for Ethylene Epoxidation. Physical Review Letters, 2010, 104, 035503.	7.8	86
137	Temperatureâ€Dependent Morphology, Magnetic and Optical Properties of Liâ€Doped MgO. ChemCatChem, 2010, 2, 854-862.	3.7	102
138	Stable structure and magnetic state of ultrathin CrAs films on GaAs(001): A density functional theory study. Physical Review B, 2010, 82, .	3.2	13
139	Role of strain in polarization switching in semipolar InGaN/GaN quantum wells. Applied Physics Letters, 2010, 97, 181102.	3.3	34
140	Coverage-Dependent Adsorption Mode of Water on Fe₃O₄(001): Insights from First Principles Calculations. Journal of Physical Chemistry C, 2010, 114, 11148-11156.	3.1	66
141	Describing Both Dispersion Interactions and Electronic Structure Using Density Functional Theory: The Case of Metalâ^'Phthalocyanine Dimers. Journal of Chemical Theory and Computation, 2010, 6, 81-90.	5.3	109
142	First-principles modeling of localized<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>states with the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi><mml:mo>@</mml:mo><mml:mtext>LDA</mml:mtext><mm Physical Review B, 2010, 82, .	3.2	222
143	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
144	Secondary Structure of Ac-Ala_n-LysH⁺ Polyalanine Peptides (n =) Tj ETQq0 0 0 rgBT /Overlock 1	4.6	76

#	Article	IF	Citations
145	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. MRS Bulletin, 2010, 35, 435-442.	3.5	257
146	First-principles study of the mechanism of ethylene epoxidation over Agâ€“Cu particles. Journal of Materials Chemistry, 2010, 20, 10521.	6.7	22
147	Large-scale surface reconstruction energetics of Pt(100) and Au(100) by all-electron density functional theory. Physical Review B, 2010, 82, .	3.2	52
148	Exploring the random phase approximation: Application to CO adsorbed on Cu(111). Physical Review B, 2009, 80, .	3.2	147
149	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 50 572 Td (stretchy="false">)	7.8	37
150	Partial Dissociation of Water on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Fe</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">O</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>001</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 532 Td (stretchy="false">)</mml	7.8	94
151	Review Letters, 2009, 103, 176102. 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:m A combined density functional theory and cluster expansion s. Physical Review B, 2009, 79, .	3.2	62
152	Dispersion-corrected MÃ¸llerâ€“Plesset second-order perturbation theory. Journal of Chemical Physics, 2009, 131, 094106.	3.0	223
153	Density functional theory study of the conformational space of an infinitely long polypeptide chain. Journal of Chemical Physics, 2009, 131, 085104.	3.0	16
154	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
155	Coupled cluster benchmarks of water monomers and dimers extracted from density-functional theory liquid water: The importance of monomer deformations. Journal of Chemical Physics, 2009, 131, 124509.	3.0	62
156	Examination of the concept of degree of rate control by first-principles kinetic Monte Carlo simulations. Surface Science, 2009, 603, 1724-1730.	1.9	99
157	Agâ€“Cu alloy surfaces in an oxidizing environment: A first-principles study. Surface Science, 2009, 603, 1467-1475.	1.9	37
158	Efficient integration for all-electron electronic structure calculation using numeric basis functions. Journal of Computational Physics, 2009, 228, 8367-8379.	3.8	454
159	Ab initio molecular simulations with numeric atom-centered orbitals. Computer Physics Communications, 2009, 180, 2175-2196.	7.5	2,170
160	Accurate Molecular Van Der Waals Interactions from Ground-State Electron Density and Free-Atom Reference Data. Physical Review Letters, 2009, 102, 073005.	7.8	4,824
161	Controlling Polarization at Insulating Surfaces: Quasiparticle Calculations for Molecules Adsorbed on Insulator Films. Physical Review Letters, 2009, 103, 056803.	7.8	65
162	Insight from first principles into the nature of the bonding between water molecules and 4d metal surfaces. Journal of Chemical Physics, 2009, 130, 184707.	3.0	94

#	Article	IF	Citations
163	Experimental and theoretical study of oxygen adsorption structures on Ag(111). Physical Review B, 2009, 80, .	3.2	90
164	Defect Formation Energies without the Band-Gap Problem: Combining Density-Functional Theory and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:math>Approach for the Silicon Self-Interstitial. Physical Review Letters, 2009, 102, 026402.	7.8	218
165	Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN. Applied Physics Letters, 2009, 95, .	3.3	151
166	Two-Step Mechanism for Low-Temperature Oxidation of Vacancies in Graphene. Physical Review Letters, 2009, 102, 166104.	7.8	122
167	Localized and Itinerant States in Lanthanide Oxides United by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi><mml:mtext>â€‰</mml:mtext><mml:mo>@</mml:mo><mml:mtext> Physical Review Letters, 2009, 102, 126403.	7.8	156
168	Compensation Mechanisms and Functionality ofÂTransition Metal Oxide Surfaces and Interfaces: AÂDensity Functional Theory Study. , 2009, , 709-717.		1
169	How strong is the bond between water and salt?. Surface Science, 2008, 602, L135-L138.	1.9	21
170	Exciting prospects for solids: Exactâ€exchange based functionals meet quasiparticle energy calculations. Physica Status Solidi (B): Basic Research, 2008, 245, 929-945.	1.5	83
171	Sources of Electrical Conductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SnO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 055502.	7.8	352
172	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
173	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters. II. The water hexamer and van der Waals interactions. Journal of Chemical Physics, 2008, 129, 194111.	3.0	211
174	Screening in two dimensions:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculations for surfaces and thin films using the repeated-slab approach. Physical Review B, 2008, 77, .	3.2	71
175	Alloy surface segregation in reactive environments: First-principles atomistic thermodynamics study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>Ag</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi>Pd</mml:mi><mml:mi> oxygen atmospheres. Physical Review B, 2008, 77, .	3.2	129
176	Nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. Physical Review B, 2008, 77, .	3.2	112
177	First-principles investigation of Ag-Cu alloy surfaces in an oxidizing environment. Physical Review B, 2008, 77, .	3.2	43
178	CO oxidation on Pd(100) at technologically relevant pressure conditions: First-principles kinetic Monte Carlo study. Physical Review B, 2008, 77, .	3.2	81
179	Influence of the Core-Valence Interaction and of the Pseudopotential Approximation on the Electron Self-Energy in Semiconductors. Physical Review Letters, 2008, 101, 106404.	7.8	107
180	Focus on Advances in Surface and Interface Science 2008. New Journal of Physics, 2008, 10, 125025.	2.9	0

#	Article	IF	Citations
181	Transition-metal silicides as materials for magnet-semiconductor heterostructures. Journal of Applied Physics, 2007, 101, 081725.	2.5	14
182	Ultrathin Oxides: Bulk-Oxide-Like Model Surfaces or Unique Films?. Physical Review Letters, 2007, 99, 086101.	7.8	53
183	First-Principles Statistical Mechanics Study of the Stability of a Subnanometer Thin Surface Oxide in Reactive Environments: CO Oxidation at Pd(100). Physical Review Letters, 2007, 98, 046101.	7.8	127
184	Towards an Exact Treatment of Exchange and Correlation in Materials: Application to the â€œCO Adsorption Puzzleâ€•and Other Systems. Physical Review Letters, 2007, 98, 176103.	7.8	110
185	Nonadiabatic potential-energy surfaces by constrained density-functional theory. Physical Review B, 2007, 75, .	3.2	85
186	Density-Functional Theory Study of Half-Metallic Heterostructures: Interstitial Mn in Si. Physical Review Letters, 2007, 98, 117202.	7.8	71
187	Density-functional study of Mn monosilicide on the Si(111) surface: Film formation versus island nucleation. Physical Review B, 2007, 76, .	3.2	30
188	Density functional theory study of flat and stepped NaCl(001). Physical Review B, 2007, 76, .	3.2	40
189	On the accuracy of density-functional theory exchange-correlation functionals for H bonds in small water clusters: Benchmarks approaching the complete basis set limit. Journal of Chemical Physics, 2007, 127, 184104.	3.0	208
190	COoxidation atPd(100): A first-principles constrained thermodynamics study. Physical Review B, 2007, 75, .	3.2	116
191	Ab initiostudy of the half-metal to metal transition in strained magnetite. New Journal of Physics, 2007, 9, 5-5.	2.9	54
192	Does phenomenological kinetics provide an adequate description of heterogeneous catalytic reactions?. Journal of Chemical Physics, 2007, 126, 204711.	3.0	120
193	Dielectric anisotropy in the GW spaceâ€“time method. Computer Physics Communications, 2007, 176, 1-13.	7.5	46
194	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
195	Structural, Electronic, and Chemical Properties of Nanoporous Carbon. Physical Review Letters, 2006, 96, 046806.	7.8	272
196	First-principles kinetic Monte Carlo simulations for heterogeneous catalysis: Application to the CO oxidation atRuO2(110). Physical Review B, 2006, 73, .	3.2	299
197	Exact-exchange-based quasiparticle energy calculations for the band gap, effective masses, and deformation potentials of ScN. Physical Review B, 2006, 74, .	3.2	89
198	Converged properties of clean metal surfaces by all-electron first-principles calculations. Surface Science, 2006, 600, 703-715.	1.9	252

#	Article	IF	Citations
199	Behler, Reuter, and Scheffler Reply:. Physical Review Letters, 2006, 96, .	7.8	5
200	â€œTextbookâ€•Adsorption at â€œNontextbookâ€•Adsorption Sites: Halogen Atoms on Alkali Halide Surfaces. Physical Review Letters, 2006, 97, 046802.	7.8	10
201	Surface reconstructions and atomic ordering inInxGa1â^'xAs(001)films: A density-functional theory study. Physical Review B, 2006, 74, .	3.2	9
202	Quantum size effect in Pb(100) films: Role of symmetry and implications for film growth. Physical Review B, 2006, 74, .	3.2	14
203	Comparison of the full-potential and frozen-core approximation approaches to density-functional calculations of surfaces. Physical Review B, 2006, 73, .	3.2	80
204	Quasiparticle Corrections to the Electronic Properties of Anion Vacancies at GaAs(110) and InP(110). Physical Review Letters, 2006, 97, 226401.	7.8	58
205	Descriptions of surface chemical reactions using a neural network representation of the potential-energy surface. Physical Review B, 2006, 73, .	3.2	113
206	Orientation-dependent surface and step energies of Pb from first principles. Physical Review B, 2006, 74, .	3.2	17
207	Density of Configurational States from First-Principles Calculations: The Phase Diagram of Al-Na Surface Alloys. ChemPhysChem, 2005, 6, 1923-1928.	2.1	20
208	Curvature effects on vacancies in nanotubes. AIP Conference Proceedings, 2005, , .	0.4	0
209	Ab initio study of transition-metal silicide films on Si(001). AIP Conference Proceedings, 2005, , .	0.4	0
210	When seeing is not believing: Oxygen on Ag(111), a simple adsorption system?. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2005, 23, 1487-1497.	2.1	108
211	First-principles study of thin magnetic transition-metal silicide films on Si(001). Physical Review B, 2005, 72, .	3.2	45
212	Xe adsorption on metal surfaces: First-principles investigations. Physical Review B, 2005, 72, .	3.2	94
213	Density-functional theory study of the initial oxygen incorporation in Pd(111). Physical Review B, 2005, 71, .	3.2	79
214	Preserving the Half-Metallicity at the Heusler AlloyCo2MnSi(001)Surface: A Density Functional Theory Study. Physical Review Letters, 2005, 94, 096402.	7.8	167
215	AB Initio Atomistic Thermodynamics and Statistical Mechanics of Surface Properties and Functions. , 2005, , 149-194.		91
216	Structural Transitions in the Polyalanine Î±-Helix under Uniaxial Strain. Journal of the American Chemical Society, 2005, 127, 17241-17244.	13.7	23

#	Article	IF	Citations
217	CombiningGWcalculations with exact-exchange density-functional theory: an analysis of valence-band photoemission for compound semiconductors. New Journal of Physics, 2005, 7, 126-126.	2.9	263
218	Jahn-Teller Stabilization of a â€œPolarâ€•Metal Oxide Surface:Fe3O4(001). Physical Review Letters, 2005, 94, 126101.	7.8	180
219	Dissociation ofO2at Al(111): The Role of Spin Selection Rules. Physical Review Letters, 2005, 94, 036104.	7.8	259
220	AB Initio Atomistic Thermodynamics and Statistical Mechanics of Surface Properties and Functions. , 2005, , 149-194.		11
221	Structure, Energetics and Properties of Fe3O4(001) from First Principles. , 2005, , 375-381.		1
222	Hydrogen adsorption onRuO2(110):â€ƒDensity-functional calculations. Physical Review B, 2004, 70, .	3.2	64
223	Adsorption and diffusion of a Cl adatom on the GaAs(001)-c(8Ã—2)Î¶surface. Physical Review B, 2004, 69, .	3.2	24
224	First-principles study of low-index surfaces of lead. Physical Review B, 2004, 70, .	3.2	57
225	A step up to self-assembly. Nature, 2004, 429, 617-618.	27.8	22
226	On the Accuracy of DFT for Describing Hydrogen Bonds:â€‰ Dependence on the Bond Directionality. Journal of Physical Chemistry A, 2004, 108, 5692-5698.	2.5	354
227	Hallmark of Perfect Graphene. Physical Review Letters, 2004, 92, 225502.	7.8	487
228	Representing high-dimensional potential-energy surfaces for reactions at surfaces by neural networks. Chemical Physics Letters, 2004, 395, 210-215.	2.6	311
229	Structure Determination of Isolated Metal Clusters via Far-Infrared Spectroscopy. Physical Review Letters, 2004, 93, 023401.	7.8	161
230	First-Principles Study of Ferromagnetism in Epitaxial Si-Mn Thin Films on Si(001). Physical Review Letters, 2004, 92, 237202.	7.8	66
231	Thermodynamic stability of PdO surfaces. Physical Review B, 2004, 69, .	3.2	193
232	The Steady State of Heterogeneous Catalysis, Studied by First-Principles Statistical Mechanics. Physical Review Letters, 2004, 93, 116105.	7.8	289
233	Oxygen Overlayers on Pd(111) Studied by Density Functional Theoryâ€. Journal of Physical Chemistry B, 2004, 108, 14477-14483.	2.6	129
234	Surface Coordination Chemistry: Dihydrogen versus Hydride Complexes on RuO2(110). Angewandte Chemie - International Edition, 2003, 42, 2151-2154.	13.8	83

#	Article	IF	Citations
235	The Pd()â€“R27Â°-O surface oxide revisited. Surface Science, 2003, 541, 101-112.	1.9	201
236	Adhesion of Copper and Alumina from First Principles. Journal of the American Ceramic Society, 2003, 86, 696-700.	3.8	21
237	Density Functional Theory Study of the Cooperativity of Hydrogen Bonds in Finite and Infinite Î±-Helices. Journal of Physical Chemistry B, 2003, 107, 1432-1437.	2.6	100
238	Why is a Noble Metal Catalytically Active? The Role of the O-Ag Interaction in the Function of Silver as an Oxidation Catalyst. Physical Review Letters, 2003, 90, 256102.	7.8	178
239	Adatom Kinetics On and Below the Surface: The Existence of a New Diffusion Channel. Physical Review Letters, 2003, 90, 056101.	7.8	293
240	Subsurface oxygen and surface oxide formation at Ag(111): A density-functional theory investigation. Physical Review B, 2003, 67, .	3.2	135
241	Nanostructures at surfaces from substrate-mediated interactions. Physical Review B, 2003, 68, .	3.2	51
242	First-Principles Atomistic Thermodynamics for Oxidation Catalysis: Surface Phase Diagrams and Catalytically Interesting Regions. Physical Review Letters, 2003, 90, 046103.	7.8	382
243	Effect of a humid environment on the surface structure ofRuO2(110). Physical Review B, 2003, 67, .	3.2	127
244	Adsorption of Xe Atoms on Metal Surfaces: New Insights from First-Principles Calculations. Physical Review Letters, 2003, 90, 066104.	7.8	168
245	Composition and structure of theRuO2(110)surface in anO2and CO environment: Implications for the catalytic formation ofCO2. Physical Review B, 2003, 68, .	3.2	442
246	Insights into the function of silver as an oxidation catalyst byab initioatomistic thermodynamics. Physical Review B, 2003, 68, .	3.2	178
247	Effect of hydrogen onAl2O3/Cuinterfacial structure and adhesion. Physical Review B, 2002, 66, .	3.2	40
248	Initial adsorption of Co on Cu(001):â€,â€,A first-principles investigation. Physical Review B, 2002, 65, .	3.2	34
249	Energy barriers and chemical properties in the coadsorption of carbon monoxide and oxygen on Ru(0001). Physical Review B, 2002, 65, .	3.2	38
250	Stability of subsurface oxygen at Rh(111). Physical Review B, 2002, 65, .	3.2	52
251	First-principles study of nucleation, growth, and interface structure of Fe/GaAs. Physical Review B, 2002, 65, .	3.2	68
252	Metastable precursors during the oxidation of the Ru(0001) surface. Physical Review B, 2002, 65, .	3.2	119

#	Article	IF	Citations
253	Comment on â€œAnomalous Mobility of Strongly Bound Surface Species: Cl onGaAs(001)-c(8Ã—2)â€• Physical Review Letters, 2002, 89, 239601; author reply 239602.	7.8	4
254	Quantum Theory of Dissociative Chemisorption on Metal Surfaces. Accounts of Chemical Research, 2002, 35, 193-200.	15.6	165
255	Oxygen adsorption on Ag(111): A density-functional theory investigation. Physical Review B, 2002, 65, .	3.2	256
256	Catalysis and corrosion: the theoretical surface-science context. Surface Science, 2002, 500, 368-394.	1.9	197
257	Quasiparticle Calculations for Point Defects on Semiconductor Surfaces. Physica Status Solidi (B): Basic Research, 2002, 234, 346-353.	1.5	8
258	Atomistic description of oxide formation on metal surfaces: the example of ruthenium. Chemical Physics Letters, 2002, 352, 311-317.	2.6	120
259	Ab Initio Thermodynamics and Statistical Mechanics of Diffusion, Growth, and Self- Assembly of Quantum Dots. , 2002, , 355-369.		1
260	Island Nucleation in Metal Thin-Film Growth. , 2002, , 87-97.		0
261	Effect of strain on surface diffusion in semiconductor heteroepitaxy. Physical Review B, 2001, 64, .	3.2	92
262	Surface core-level shifts at an oxygen-rich Ru surface: O/Ru(0001) vs. RuO2(110). Surface Science, 2001, 490, 20-28.	1.9	55
263	Composition, structure, and stability ofRuO2(110)as a function of oxygen pressure. Physical Review B, 2001, 65, .	3.2	1,771
264	The CO/Pt(111) Puzzle. Journal of Physical Chemistry B, 2001, 105, 4018-4025.	2.6	642
265	Exchange-correlation kernels for excited states in solids. Physical Review B, 2001, 63, .	3.2	25
266	Substrate-Mediated Interaction on Ag(111) Surfaces from First Principles. NATO Science Series Series II, Mathematics, Physics and Chemistry, 2001, , 225-236.	0.1	2
267	Improving the efficiency of FP-LAPW calculations. Computer Physics Communications, 2000, 126, 294-309.	7.5	252
268	GaAs(001) Surface under Conditions of Low As Pressure: Evidence for a Novel Surface Geometry. Physical Review Letters, 2000, 85, 3890-3893.	7.8	189
269	Island Nucleation in Thin-Film Epitaxy: A First-Principles Investigation. Physical Review Letters, 2000, 84, 5371-5374.	7.8	226
270	Dynamics of hydrogen dissociation at the sulfur-covered Pd(100) surface. Physical Review B, 2000, 61, 8425-8432.	3.2	32

#	Article	IF	Citations
271	Energetics of InAs Thin Films and Islands on the GaAs(001) Substrate. Japanese Journal of Applied Physics, 2000, 39, 4298-4301.	1.5	17
272	Effect of the Environment onÎ±â^'Al2O3(0001) Surface Structures. Physical Review Letters, 2000, 84, 3650-3653.	7.8	473
273	Ab InitioBased Tight-Binding Hamiltonian for the Dissociation of Molecules at Surfaces. Physical Review Letters, 1999, 82, 1209-1212.	7.8	36
274	Trends in the chemical reactivity of surfaces studied byab initioquantum-dynamics calculations. Physical Review B, 1999, 59, 13297-13300.	3.2	67
275	Rotational effects in the dissociation of H2 on metal surfaces studied by ab initio quantum-dynamics calculations. Chemical Physics Letters, 1999, 311, 1-7.	2.6	32
276	Ab initio pseudopotentials for electronic structure calculations of poly-atomic systems using density-functional theory. Computer Physics Communications, 1999, 119, 67-98.	7.5	1,313
277	Phonon- Versus Electron-Mediated Desorption and Oxidation of CO on Ru(0001). Science, 1999, 285, 1042-1045.	12.6	443
278	Temperature-dependent surface relaxations of Ag(111). Physical Review B, 1999, 59, 970-974.	3.2	58
279	The adsorption of oxygen at GaN surfaces. Applied Physics Letters, 1999, 74, 1695-1697.	3.3	219
280	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
281	First-Principles Theory of Surface Thermodynamics and Kinetics. Physical Review Letters, 1999, 83, 2993-2996.	7.8	181
282	First-principles calculation of the thermal properties of silver. Physical Review B, 1999, 59, 965-969.	3.2	124
283	Density-functional theory studies on microscopic processes of gaas growth. Progress in Surface Science, 1998, 59, 135-147.	8.3	22
284	Adatom diffusion at GaN (0001) and (000Ì„) surfaces. Applied Physics Letters, 1998, 73, 487-489.	3.3	436
285	Influence of surface stress on the equilibrium shape of strained quantum dots. Physical Review B, 1998, 58, 4566-4571.	3.2	192
286	Pseudopotential study of binding properties of solids within generalized gradient approximations: The role of core-valence exchange correlation. Physical Review B, 1998, 57, 2134-2145.	3.2	197
287	The Hematite (Î±- Fe2O3) (0001) Surface: Evidence for Domains of Distinct Chemistry. Physical Review Letters, 1998, 81, 1038-1041.	7.8	490
288	Island morphology and adatom self-diffusion on Pt(111). Physical Review B, 1998, 57, 1881-1889.	3.2	90

#	Article	IF	Citations
289	Structure and dynamics of Rh surfaces. Physical Review B, 1998, 57, 4768-4775.	3.2	25
290	Ab initioquantum and molecular dynamics of the dissociative adsorption of hydrogen on Pd(100). Physical Review B, 1998, 57, 2493-2506.	3.2	158
291	Clean and As-Covered Zinc-Blende GaN (001) Surfaces: Novel Surface Structures and Surfactant Behavior. Physical Review Letters, 1998, 80, 3097-3100.	7.8	99
292	Coadsorption of CO and O on Ru(0001): A Structural Analysis by Density Functional Theory. Israel Journal of Chemistry, 1998, 38, 409-414.	2.3	10
293	Steering and Isotope Effects in the Dissociative Adsorption of H2/Pd(100). , 1998, , 285-292.		1
294	Ab initiostudy of the anomalies in the He-atom-scattering spectra of H/Mo(110) and H/W(110). Physical Review B, 1997, 56, 13503-13518.	3.2	34
295	Novel Diffusion Mechanism on the GaAs(001) Surface: The Role of Adatom-Dimer Interaction. Physical Review Letters, 1997, 79, 5278-5281.	7.8	175
296	Surface Relaxation and Ferromagnetism of Rh(001). Physical Review Letters, 1997, 78, 1299-1302.	7.8	70
297	Hydrogen-Induced Polymorphism of the Pd(110) Surface. Physical Review Letters, 1997, 79, 1329-1332.	7.8	25
298	Role of zero-point effects in catalytic reactions involving hydrogen. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1997, 15, 1624-1629.	2.1	57
299	Strain dependence of surface diffusion: Ag on Ag(111) and Pt(111). Physical Review B, 1997, 55, 6750-6753.	3.2	171
300	Ab initio study of step formation and self-diffusion on Ag(100). Physical Review B, 1997, 55, 13916-13924.	3.2	66
301	Theory of Self-Diffusion in GaAs*. Zeitschrift Fur Physikalische Chemie, 1997, 200, 195-207.	2.8	33
302	A Model for the Thermal Expansion of Ag(111) and other Metal Surfaces. Zeitschrift Fur Physikalische Chemie, 1997, 202, 253-262.	2.8	26
303	Ab InitioMolecular Dynamics Study of the Desorption ofD2from Si(100). Physical Review Letters, 1997, 79, 701-704.	7.8	67
304	Physical origin of exchange diffusion on fcc(100) metal surfaces. Physical Review B, 1997, 56, R15569-R15572.	3.2	104
305	Density-functional theory calculations for poly-atomic systems: electronic structure, static and elastic properties and ab initio molecular dynamics. Computer Physics Communications, 1997, 107, 187-222.	7.5	660
306	Six-dimensional quantum dynamics of adsorption and desorption of H2 at Pd(100): no need for a molecular precursor adsorption state. Surface Science, 1996, 357-358, 614-618.	1.9	43

#	Article	IF	Citations
307	Anomalies in He atom scattering spectra of the H-covered Mo(110) and W(110) surfaces. Surface Science, 1996, 368, 213-221.	1.9	15
308	Abinitiopseudopotential study of Fe, Co, and Ni employing the spin-polarized LAPW approach. Physical Review B, 1996, 53, 10685-10689.	3.2	53
309	Structure and Stability of a High-Coverage(1Ã—1)Oxygen Phase on Ru(0001). Physical Review Letters, 1996, 77, 3371-3374.	7.8	220
310	Abinitiocalculations of energies and self-diffusion on flat and stepped surfaces of Al and their implications on crystal growth. Physical Review B, 1996, 53, 4958-4973.	3.2	212
311	Anisotropy of Growth of the Close-Packed Surfaces of Silver. Physical Review Letters, 1996, 77, 1095-1098.	7.8	133
312	Enhanced Electron-Phonon Coupling at the Mo and W(110) Surfaces Induced by Adsorbed Hydrogen. Zeitschrift Fur Physikalische Chemie, 1996, 197, 193-202.	2.8	17
313	Influence of molecular vibrations on dissociative adsorption. Chemical Physics Letters, 1996, 256, 417-423.	2.6	65
314	Force calculation and atomic-structure optimization for the full-potential linearized augmented plane-wave code WIEN. Computer Physics Communications, 1996, 94, 31-48.	7.5	177
315	Scattering of hydrogen molecules from a reactive surface: Strong off-specular and rotationally inelastic diffraction. Chemical Physics Letters, 1996, 263, 567-573.	2.6	43
316	GaAs equilibrium crystal shape from first principles. Physical Review B, 1996, 54, 8844-8855.	3.2	383
317	Theoretical study of O adlayers on Ru(0001). Physical Review B, 1996, 54, 2868-2872.	3.2	160
318	Gross and Scheffler Reply:. Physical Review Letters, 1996, 77, 405-405.	7.8	32
319	Local Isoelectronic Reactivity of Solid Surfaces. Physical Review Letters, 1996, 77, 1560-1563.	7.8	48
320	Homoepitaxial Growth of Metals and the Role of Surfactants. , 1996, , 219-231.		0
321	Green function for crystal surfaces I. Computer Physics Communications, 1995, 88, 230-248.	7.5	2
322	Six-Dimensional Quantum Dynamics of Adsorption and Desorption ofH2at Pd(100): Steering and Steric Effects. Physical Review Letters, 1995, 75, 2718-2721.	7.8	358
323	Frustrated H-Induced Instability of Mo(110). Physical Review Letters, 1995, 74, 1387-1390.	7.8	69
324	Frustrated H-Induced Instability of Mo(110). Physical Review Letters, 1995, 75, 1681-1681.	7.8	0

#	Article	IF	Citations
325	Local Chemical Reactivity of a Metal Alloy Surface. Physical Review Letters, 1995, 74, 3487-3490.	7.8	210
326	Localized Excitons and Breaking of Chemical Bonds at III-V (110) Surfaces. Physical Review Letters, 1995, 75, 701-704.	7.8	45
327	THEORY OF ALKALI-METAL ADSORPTION ON CLOSE-PACKED METAL SURFACES. Surface Review and Letters, 1995, 02, 317-343.	1.1	76
328	Poisoning of Pd(100) for the dissociation of H2: a theoretical study of co-adsorption of hydrogen and sulphur. Surface Science, 1995, 329, L605-L610.	1.9	85
329	Theory of Self-Diffusion at and Growth of A1(111). Physical Review Letters, 1994, 73, 508-508.	7.8	7
330	Surface core-level shifts of some 4d-metal single-crystal surfaces: Experiments andabinitiocalculations. Physical Review B, 1994, 50, 17525-17533.	3.2	201
331	High-Dimensional Quantum Dynamics of Adsorption and Desorption ofH2at Cu(111). Physical Review Letters, 1994, 73, 3121-3124.	7.8	145
332	Theory of self-diffusion at and growth of Al(111). Physical Review Letters, 1994, 72, 254-257.	7.8	231
333	Simultaneous calculation of the equilibrium atomic structure and its electronic ground state using density-functional theory. Computer Physics Communications, 1994, 79, 447-465.	7.5	249
334	A self-consistent surface Green-function (SSGF) method for the calculation of isolated adsorbate atoms on a semi-infinite crystal. Computer Physics Communications, 1994, 79, 124-142.	7.5	5
335	Mechanisms of self-diffusion on flat and stepped Al surfaces. Surface Science, 1994, 307-309, 501-506.	1.9	15
336	Surface polarons and bipolarons at GaAs(110) with adsorbed alkali metals. Surface Science, 1994, 307-309, 1001-1006.	1.9	6
337	Thick sodium overlayers on GaAs(110). Physical Review B, 1994, 49, 5516-5521.	3.2	4
338	Multidimensional Potential Energy Surface forH2Dissociation over Cu(111). Physical Review Letters, 1994, 73, 1400-1403.	7.8	334
339	Reconstruction mechanism of fcc transition metal (001) surfaces. Physical Review Letters, 1993, 71, 1051-1054.	7.8	262
340	Electronic structure of R30Â°-Na and -K on Al(111): Comparison of â€œnormalâ€•and substitutional adsorption sites. Surface Science, 1993, 287-288, 559-563.	1.9	17
341	Theory of adsorption and desorption in high electric fields. Surface Science, 1993, 287-288, 572-576.	1.9	44
342	Electron correlations on a potassium-covered GaAs(110) surface: ab-initio calculations of the Hubbard correlation energy. Surface Science, 1993, 287-288, 584-587.	1.9	10

#	Article	IF	Citations
343	Bound bipolaron at the surface: The negative-Ubehavior of GaAs(110) with adsorbed alkali metals. Physical Review Letters, 1993, 71, 2797-2800.	7.8	44
344	Electronic and structural properties of GaN by the full-potential linear muffin-tin orbitals method: The role of thedelectrons. Physical Review B, 1993, 47, 13353-13362.	3.2	188
345	Hubbard correlations and charge transfer at the GaAs(110) surface with alkali adsorbates. Physical Review Letters, 1993, 70, 351-354.	7.8	70
346	Theory of adsorption and surfactant effect of Sb on Ag(111). Physical Review Letters, 1993, 71, 2437-2440.	7.8	134
347	Mechanisms of island formation of alkali-metal adsorbates on Al(111). Physical Review Letters, 1993, 71, 577-580.	7.8	129
348	Pressure dependence of deep levels of the As antisite, the Ga-vacancyâ€“As-interstitial pair, and of the stable and metastable states ofEL2. Physical Review B, 1993, 47, 16624-16627.	3.2	13
349	Evidence for site-sensitive screening of core holes at the Si and Ge (001) surface. Physical Review Letters, 1993, 71, 2338-2341.	7.8	377
350	Chapter 1 Density-Functional Theory of sp-Bonded Defects in III/V Semiconductors. Semiconductors and Semimetals, 1993, , 1-58.	0.7	12
351	Surface Alloying and Surfactant Action of Sb ON Ag (111). Materials Research Society Symposia Proceedings, 1993, 317, 323.	0.1	1
352	Defect Metastability in III-V Compounds. Materials Science Forum, 1992, 83-87, 735-750.	0.3	42
353	Self-consistent pseudopotential calculations for sodium adsorption on GaAs(110). Physical Review B, 1992, 46, 10134-10145.	3.2	49
354	Adsorbate-substrate and adsorbate-adsorbate interactions of Na and K adlayers on Al(111). Physical Review B, 1992, 46, 16067-16080.	3.2	2,339
355	Trends of the surface relaxations, surface energies, and work functions of the 4dtransition metals. Physical Review B, 1992, 46, 4816-4829.	3.2	532
356	Self-consistent study of the electronic and structural properties of the clean Si(001)(2 Ã— 1) surface. Applied Surface Science, 1992, 56-58, 15-19.	6.1	250
357	Formation energies and abundances of intrinsic point defects at the GaAs/AlAs(100) interface. Applied Surface Science, 1992, 56-58, 628-631.	6.1	6
358	Calculated atomic structures and electronic properties of GaP, InP, GaAs, and InAs (110) surfaces. Physical Review B, 1991, 44, 6188-6198.	3.2	219
359	Analysis of separable potentials. Physical Review B, 1991, 44, 8503-8513.	3.2	508
360	Unusual chemisorption geometry of Na on Al(111). Physical Review Letters, 1991, 67, 2163-2166.	7.8	191

#	Article	IF	Citations
361	Atomic and electronic structures of GaAs(110) and their alkali-adsorption-induced changes. Physical Review Letters, 1991, 67, 1031-1034.	7.8	92
362	Ghost states for separable, norm-conserving, Iab initioP pseudopotentials. Physical Review B, 1990, 41, 12264-12267.	3.2	155
363	Negative thermal expansion of diamond and zinc-blende semiconductors. Physical Review Letters, 1989, 63, 290-293.	7.8	147
364	Isolated arsenic-antisite defect in GaAs and the properties ofEL2. Physical Review B, 1989, 40, 10391-10401.	3.2	172
365	Chemical binding, stability and metastability of defects in semiconductors. FestkÃ¶rperprobleme, 1989, , 231-250.	0.7	7
366	The EL2 Defect in GaAs. Materials Science Forum, 1989, 38-41, 51-58.	0.3	15
367	Surface green's function for a rumpled crystal surface. Computer Physics Communications, 1988, 51, 381-390.	7.5	12
368	Electronic structure of fcc and bcc close-packed silver surfaces. Physical Review B, 1988, 38, 8505-8507.	3.2	17
369	Parameter-free calculations of total energies, interatomic forces and vibrational entropies of defects in semiconductors. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1988, 58, 107-121.	0.6	99
370	Theoretical Evidence for an Optically Inducible Structural Transition of the Isolated As Antisite in GaAs: Identification and Explanation ofEL2?. Physical Review Letters, 1988, 60, 2183-2186.	7.8	267
371	Thermodynamic Aspects of Bulk and Surface Defectsâ€“First-Principle Calculations -. Studies in Surface Science and Catalysis, 1988, 40, 115-122.	1.5	5
372	Mechanisms of defect pairing in semiconductors: A study for chalcogens in silicon. Physical Review Letters, 1987, 58, 1456-1459.	7.8	32
373	A new version of the program for the calculation of the green's function for a crystal surface or interface. Computer Physics Communications, 1987, 47, 349-350.	7.5	8
374	Lattice relaxations at substitutional impurities in semiconductors. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1987, 146, 176-186.	0.9	41
375	LATTICE RELAXATIONS AT SUBSTITUTIONAL IMPURITIES IN SEMICONDUCTORS. , 1987, , 176-186.		0
376	Resonant Raman Scattering at Point Defects in GaAs. Materials Science Forum, 1986, 10-12, 353-358.	0.3	12
377	Chalcogen and Vacancy Pairs in Silicon: Electronic Structure and Stabilities. Materials Science Forum, 1986, 10-12, 25-30.	0.3	39
378	Calculation of the green's function for a crystal surface or interface. Computer Physics Communications, 1985, 38, 403-413.	7.5	33

#	Article	IF	Citations
379	Identification of Chalcogen Point-Defect Sites in Silicon by Total-Energy Calculations. Physical Review Letters, 1985, 54, 2525-2528.	7.8	52
380	Total-energy gradients and lattice distortions at point defects in semiconductors. Physical Review B, 1985, 31, 6541-6551.	3.2	125
381	The adsorption of sulphur on Pd(111) I. A LEED analysis of the adsorbate structure. Surface Science, 1985, 160, 467-474.	1.9	58
382	Angle-resolved photoemission and the electronic structure of Pd(111). Physical Review B, 1984, 29, 692-702.	3.2	46
383	Tractable Approach for Calculating Lattice Distortions around Simple Defects in Semiconductors: Application to the Single Donor Ge in GaP. Physical Review Letters, 1982, 49, 1765-1768.	7.8	55
384	Electronic structure of simple deep-level defects in semiconductors. , 1982, , 115-148.		10
385	The influence of lateral interactions on the vibrational spectrum of adsorbed CO. Surface Science, 1979, 81, 562-570.	1.9	225
386	Quasiparticle Calculations for Point Defects at Semiconductor Surfaces. Topics in Applied Physics, 0, , 165-192.	0.8	1