Matthias Scheffler

List of Publications by Citations

376 papers	48,326 citations	115 h-index	211 g-index
398 ext. papers	52,562 ext. citations	5.5 avg, IF	7.86 L-index

#	Paper	IF	Citations
376	Accurate molecular van der Waals interactions from ground-state electron density and free-atom reference data. *Physical Review Letters*, **2009**, 102, 073005	7.4	3885
375	Adsorbate-substrate and adsorbate-adsorbate interactions of Na and K adlayers on Al(111). *Physical Review B*, **1992**, 46, 16067-16080	3.3	1987
374	Ab initio molecular simulations with numeric atom-centered orbitals. *Computer Physics Communications*, **2009**, 180, 2175-2196	4.2	1637
373	Composition, structure, and stability of RuO2(110) as a function of oxygen pressure. *Physical Review B*, **2001**, 65,	3.3	1561
372	Ab initio pseudopotentials for electronic structure calculations of poly-atomic systems using density-functional theory. *Computer Physics Communications*, **1999**, 119, 67-98	4.2	1174
371	Accurate and efficient method for many-body van der Waals interactions. *Physical Review Letters*, **2012**, 108, 236402	7.4	920
370	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
369	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	4.2	628
368	The CO/Pt(111) Puzzle. *Journal of Physical Chemistry B*, **2001**, 105, 4018-4025	3.4	579
367	CO oxidation as a prototypical reaction for heterogeneous processes. *Angewandte Chemie - International Edition*, **2011**, 50, 10064-94	16.4	510
366	Big data of materials science: critical role of the descriptor. *Physical Review Letters*, **2015**, 114, 105503	7.4	495
365	Trends of the surface relaxations, surface energies, and work functions of the 4d transition metals. *Physical Review B*, **1992**, 46, 4816-4829	3.3	490
364	Density-functional theory with screened van der Waals interactions for the modeling of hybrid inorganic-organic systems. *Physical Review Letters*, **2012**, 108, 146103	7.4	467
363	Analysis of separable potentials. *Physical Review B*, **1991**, 44, 8503-8513	3.3	466
362	The Hematite (□Fe2O3) (0001) Surface: Evidence for Domains of Distinct Chemistry. *Physical Review Letters*, **1998**, 81, 1038-1041	7.4	447
361	Hallmark of perfect graphene. *Physical Review Letters*, **2004**, 92, 225502	7.4	440
360	Effect of the environment on alpha-Al2O3 (0001) surface structures. *Physical Review Letters*, **2000**, 84, 3650-3	7.4	430

359	Resolution-of-identity approach to Hartree–Fock, hybrid density functionals, RPA, MP2 and GW with numeric atom-centered orbital basis functions. *New Journal of Physics*, **2012**, 14, 053020	2.9	411
358	Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies. *Journal of Chemical Theory and Computation*, **2013**, 9, 3404-19	6.4	410
357	Composition and structure of the RuO2(110) surface in an O2 and CO environment: Implications for the catalytic formation of CO2. *Physical Review B*, **2003**, 68,	3.3	401
356	Adatom diffusion at GaN (0001) and (000$\bar{1}$) surfaces. *Applied Physics Letters*, **1998**, 73, 487-489	3.4	400
355	Phonon- versus electron-mediated desorption and oxidation of CO on Ru(0001). *Science*, **1999**, 285, 1042-5	33.3	395
354	Random-phase approximation and its applications in computational chemistry and materials science. *Journal of Materials Science*, **2012**, 47, 7447-7471	4.3	389
353	New tolerance factor to predict the stability of perovskite oxides and halides. *Science Advances*, **2019**, 5, eaav0693	14.3	376
352	GaAs equilibrium crystal shape from first principles. *Physical Review B*, **1996**, 54, 8844-8855	3.3	366
351	Evidence for site-sensitive screening of core holes at the Si and Ge (001) surface. *Physical Review Letters*, **1993**, 71, 2338-2341	7.4	350
350	First-principles atomistic thermodynamics for oxidation catalysis: surface phase diagrams and catalytically interesting regions. *Physical Review Letters*, **2003**, 90, 046103	7.4	344
349	Efficient O(N) integration for all-electron electronic structure calculation using numeric basis functions. *Journal of Computational Physics*, **2009**, 228, 8367-8379	4.1	342
348	Six-dimensional quantum dynamics of adsorption and desorption of H2 at Pd(100): Steering and steric effects. *Physical Review Letters*, **1995**, 75, 2718-2721	7.4	338
347	On the Accuracy of DFT for Describing Hydrogen Bonds: Dependence on the Bond Directionality. *Journal of Physical Chemistry A*, **2004**, 108, 5692-5698	2.8	324
346	Multidimensional potential energy surface for H2 dissociation over Cu(111). *Physical Review Letters*, **1994**, 73, 1400-1403	7.4	313
345	Sources of electrical conductivity in SnO2. *Physical Review Letters*, **2008**, 101, 055502	7.4	309
344	Understanding band gaps of solids in generalized Kohn-Sham theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2801-2806	11.5	280
343	Adatom kinetics on and below the surface: the existence of a new diffusion channel. *Physical Review Letters*, **2003**, 90, 056101	7.4	267
342	The steady state of heterogeneous catalysis, studied by first-principles statistical mechanics. *Physical Review Letters*, **2004**, 93, 116105	7.4	265

341	First-principles kinetic Monte Carlo simulations for heterogeneous catalysis: Application to the CO oxidation at RuO2(110). *Physical Review B*, **2006**, 73,	3.3	264
340	Representing high-dimensional potential-energy surfaces for reactions at surfaces by neural networks. *Chemical Physics Letters*, **2004**, 395, 210-215	2.5	262
339	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	250
338	Structural, electronic, and chemical properties of nanoporous carbon. *Physical Review Letters*, **2006**, 96, 046806	7.4	250
337	Reconstruction mechanism of fcc transition metal (001) surfaces. *Physical Review Letters*, **1993**, 71, 1051-1054	7.4	249
336	Theoretical evidence for an optically inducible structural transition of the isolated As antisite in GaAs: Identification and explanation of EL2?. *Physical Review Letters*, **1988**, 60, 2183-2186	7.4	249
335	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. *MRS Bulletin*, **2010**, 35, 435-442	3.2	244
334	Simultaneous calculation of the equilibrium atomic structure and its electronic ground state using density-functional theory. *Computer Physics Communications*, **1994**, 79, 447-465	4.2	244
333	Self-consistent study of the electronic and structural properties of the clean Si(001)(2 □1) surface. *Applied Surface Science*, **1992**, 56-58, 15-19	6.7	241
332	Dissociation of O2 at Al(111): the role of spin selection rules. *Physical Review Letters*, **2005**, 94, 036104	7.4	234
331	Oxygen adsorption on Ag(111): A density-functional theory investigation. *Physical Review B*, **2002**, 65,	3.3	231
330	Dispersion Interactions with Density-Functional Theory: Benchmarking Semiempirical and Interatomic Pairwise Corrected Density Functionals. *Journal of Chemical Theory and Computation*, **2011**, 7, 3944-51	6.4	230
329	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. *Physical Review B*, **2012**, 86,	3.3	227
328	Converged properties of clean metal surfaces by all-electron first-principles calculations. *Surface Science*, **2006**, 600, 703-715	1.8	225
327	Theory of self-diffusion at and growth of Al(111). *Physical Review Letters*, **1994**, 72, 254-257	7.4	220
326	Island nucleation in thin-film epitaxy: A first-principles investigation. *Physical Review Letters*, **2000**, 84, 5371-4	7.4	215
325	Structure and Stability of a High-Coverage (1 x 1) Oxygen Phase on Ru(0001). *Physical Review Letters*, **1996**, 77, 3371-3374	7.4	209
324	Calculated atomic structures and electronic properties of GaP, InP, GaAs, and InAs (110) surfaces. *Physical Review B*, **1991**, 44, 6188-6198	3.3	209

323	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
322	The influence of lateral interactions on the vibrational spectrum of adsorbed CO. *Surface Science*, **1979**, 81, 562-570	1.8	207
321	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	3.9	204
320	Ab initio calculations 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	3.3	204
319	The adsorption of oxygen at GaN surfaces. *Applied Physics Letters*, **1999**, 74, 1695-1697	3.4	197
318	Defect formation energies without the band-gap problem: combining density-functional theory and the GW approach for the silicon self-interstitial. *Physical Review Letters*, **2009**, 102, 026402	7.4	196
317	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	3.9	195
316	Surface core-level shifts of some 4d-metal single-crystal surfaces: Experiments and ab initio calculations. *Physical Review B*, **1994**, 50, 17525-17533	3.3	189
315	First-principles modeling of localized d states with the GW@LDA+U approach. *Physical Review B*, **2010**, 82,	3.3	188
314	GaAs(001) surface under conditions of low As pressure: evidence for a novel surface geometry. *Physical Review Letters*, **2000**, 85, 3890-3	7.4	187
313	Catalysis and corrosion: the theoretical surface-science context. *Surface Science*, **2002**, 500, 368-394	1.8	186
312	The Pd()R27°-O surface oxide revisited. *Surface Science*, **2003**, 541, 101-112	1.8	185
311	Influence of surface stress on the equilibrium shape of strained quantum dots. *Physical Review B*, **1998**, 58, 4566-4571	3.3	183
310	Hydrogen bonds and van der waals forces in ice at ambient and high pressures. *Physical Review Letters*, **2011**, 107, 185701	7.4	181
309	Improving the efficiency of FP-LAPW calculations. *Computer Physics Communications*, **2000**, 126, 294-309	4.2	181
308	Unusual chemisorption geometry of Na on Al(111). *Physical Review Letters*, **1991**, 67, 2163-2166	7.4	180
307	Local Chemical Reactivity of a Metal Alloy Surface. *Physical Review Letters*, **1995**, 74, 3487-3490	7.4	179
306	Modeling adsorption and reactions of organic molecules at metal surfaces. *Accounts of Chemical Research*, **2014**, 47, 3369-77	24.3	177

305	Electronic and structural properties of GaN by the full-potential linear muffin-tin orbitals method: The role of the d electrons. *Physical Review B*, **1993**, 47, 13353-13362	3.3	177
304	A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane. *Catalysis Reviews - Science and Engineering*, **2011**, 53, 424-514	12.6	174
303	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	3.3	174
302	Dispersion-corrected Mller-Plesset second-order perturbation theory. *Journal of Chemical Physics*, **2009**, 131, 094106	3.9	172
301	Beyond the random-phase approximation for the electron correlation energy: the importance of single excitations. *Physical Review Letters*, **2011**, 106, 153003	7.4	171
300	Jahn-Teller stabilization of a "polar" metal oxide surface: Fe3O4(001). *Physical Review Letters*, **2005**, 94, 126101	7.4	170
299	Thermodynamic stability of PdO surfaces. *Physical Review B*, **2004**, 69,	3.3	170
298	SISSO: A compressed-sensing method for identifying the best low-dimensional descriptor in an immensity of offered candidates. *Physical Review Materials*, **2018**, 2,	3.2	170
297	Force calculation and atomic-structure optimization for the full-potential linearized augmented plane-wave code WIEN. *Computer Physics Communications*, **1996**, 94, 31-48	4.2	167
296	First-Principles Theory of Surface Thermodynamics and Kinetics. *Physical Review Letters*, **1999**, 83, 2993-2996	7.4	166
295	Novel Diffusion Mechanism on the GaAs(001) Surface: The Role of Adatom-Dimer Interaction. *Physical Review Letters*, **1997**, 79, 5278-5281	7.4	163
294	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	7.4	158
293	Adsorption of Xe atoms on metal surfaces: new insights from first-principles calculations. *Physical Review Letters*, **2003**, 90, 066104	7.4	158
292	Electronic band structure of zirconia and hafnia polymorphs from the GW perspective. *Physical Review B*, **2010**, 81,	3.3	157
291	Insights into the function of silver as an oxidation catalyst by ab initio atomistic thermodynamics. *Physical Review B*, **2003**, 68,	3.3	157
290	Strain dependence of surface diffusion: Ag on Ag(111) and Pt(111). *Physical Review B*, **1997**, 55, 6750-6753	3.3	155
289	NOMAD: The FAIR concept for big data-driven materials science. *MRS Bulletin*, **2018**, 43, 676-682	3.2	155
288	Quantum theory of dissociative chemisorption on metal surfaces. *Accounts of Chemical Research*, **2002**, 35, 193-200	24.3	154

287	Isolated arsenic-antisite defect in GaAs and the properties of EL2. *Physical Review B*, **1989**, 40, 10391-10401	3.3	154
286	Preserving the half-metallicity at the Heusler alloy Co2MnSi(001) surface: a density functional theory study. *Physical Review Letters*, **2005**, 94, 096402	7.4	152
285	Insightful classification of crystal structures using deep learning. *Nature Communications*, **2018**, 9, 2775	17.4	151
284	Structure determination of isolated metal clusters via far-infrared spectroscopy. *Physical Review Letters*, **2004**, 93, 023401	7.4	148
283	Ab initio quantum and molecular dynamics of the dissociative adsorption of hydrogen on Pd(100). *Physical Review B*, **1998**, 57, 2493-2506	3.3	148
282	Atomic Structure of the GaAs(001)[2×4] Surface Resolved Using Scanning Tunneling Microscopy and First-Principles Theory. *Physical Review Letters*, **1999**, 83, 2989-2992	7.4	148
281	Theoretical study of O adlayers on Ru(0001). *Physical Review B*, **1996**, 54, 2868-2872	3.3	147
280	Ghost states for separable, norm-conserving, Iab initioP pseudopotentials. *Physical Review B*, **1990**, 41, 12264-12267	3.3	145
279	Localized and itinerant states in lanthanide oxides united by GW @ LDA+U. *Physical Review Letters*, **2009**, 102, 126403	7.4	142
278	Exploring the random phase approximation: Application to CO adsorbed on Cu(111). *Physical Review B*, **2009**, 80,	3.3	136
277	Negative thermal expansion of diamond and zinc-blende semiconductors. *Physical Review Letters*, **1989**, 63, 290-293	7.4	133
276	Benchmark of GW methods for azabenzenes. *Physical Review B*, **2012**, 86,	3.3	132
275	Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN. *Applied Physics Letters*, **2009**, 95, 121111	3.4	132
274	First-principles optical spectra for F centers in MgO. *Physical Review Letters*, **2012**, 108, 126404	7.4	131
273	Van der Waals interactions in ionic and semiconductor solids. *Physical Review Letters*, **2011**, 107, 245501	7.4	131
272	High-dimensional quantum dynamics of adsorption and desorption of H2 at Cu(111). *Physical Review Letters*, **1994**, 73, 3121-3124	7.4	131
271	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	129
270	Anisotropy of Growth of the Close-Packed Surfaces of Silver. *Physical Review Letters*, **1996**, 77, 1095-1098	7.4	128

269	Subsurface oxygen and surface oxide formation at Ag(111): A density-functional theory investigation. *Physical Review B*, **2003**, 67,	3.3	127
268	Mechanisms of island formation of alkali-metal adsorbates on Al(111). *Physical Review Letters*, **1993**, 71, 577-580	7.4	126
267	Theory of adsorption and surfactant effect of Sb on Ag(111). *Physical Review Letters*, **1993**, 71, 2437-2440	7.4	123
266	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	7.4	121
265	Self-consistent GW: All-electron implementation with localized basis functions. *Physical Review B*, **2013**, 88,	3.3	120
264	Total-energy gradients and lattice distortions at point defects in semiconductors. *Physical Review B*, **1985**, 31, 6541-6551	3.3	120
263	Alloy surface segregation in reactive environments: First-principles atomistic thermodynamics study of Ag3Pd(111) in oxygen atmospheres. *Physical Review B*, **2008**, 77,	3.3	119
262	Effect of a humid environment on the surface structure of RuO2(110). *Physical Review B*, **2003**, 67,	3.3	117
261	Oxygen Overlayers on Pd(111) Studied by Density Functional Theory *Journal of Physical Chemistry B*, **2004**, 108, 14477-14483	3.4	112
260	Metastable precursors during the oxidation of the Ru(0001) surface. *Physical Review B*, **2002**, 65,	3.3	112
259	Assessment of correlation energies based on the random-phase approximation. *New Journal of Physics*, **2012**, 14, 043002	2.9	111
258	Atomistic description of oxide formation on metal surfaces: the example of ruthenium. *Chemical Physics Letters*, **2002**, 352, 311-317	2.5	111
257	Performance of various density-functional approximations for cohesive properties of 64 bulk solids. *New Journal of Physics*, **2018**, 20, 063020	2.9	110
256	First-principles calculation of the thermal properties of silver. *Physical Review B*, **1999**, 59, 965-969	3.3	109
255	Does phenomenological kinetics provide an adequate description of heterogeneous catalytic reactions?. *Journal of Chemical Physics*, **2007**, 126, 204711	3.9	108
254	Role of nitrogen vacancies in the luminescence of Mg-doped GaN. *Applied Physics Letters*, **2012**, 100, 142110	3.4	107
253	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	3.9	107
252	Two-step mechanism for low-temperature oxidation of vacancies in graphene. *Physical Review Letters*, **2009**, 102, 166104	7.4	106

251	CO oxidation at Pd(100): A first-principles constrained thermodynamics study. *Physical Review B*, **2007**, 75,	3.3	106
250	Magnetism in C- or N-doped MgO and ZnO: a density-functional study of impurity pairs. *Physical Review Letters*, **2010**, 105, 267203	7.4	103
249	Physical origin of exchange diffusion on fcc(100) metal surfaces. *Physical Review B*, **1997**, 56, R15569-R15572	3.3	103
248	Nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. *Physical Review B*, **2008**, 77,	3.3	103
247	Descriptions of surface chemical reactions using a neural network representation of the potential-energy surface. *Physical Review B*, **2006**, 73,	3.3	103
246	Towards an exact treatment of exchange and correlation in materials: application to the "CO adsorption puzzle" and other systems. *Physical Review Letters*, **2007**, 98, 176103	7.4	102
245	Describing Both Dispersion Interactions and Electronic Structure Using Density Functional Theory: The Case of Metal-Phthalocyanine Dimers. *Journal of Chemical Theory and Computation*, **2010**, 6, 81-90	6.4	100
244	Hybrid density functional theory meets quasiparticle calculations: A consistent electronic structure approach. *Physical Review B*, **2013**, 88,	3.3	99
243	Density Functional Theory Study of the Cooperativity of Hydrogen Bonds in Finite and Infinite -Helices. *Journal of Physical Chemistry B*, **2003**, 107, 1432-1437	3.4	99
242	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	2.9	97
241	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,	3.3	96
240	Beyond Scaling Relations for the Description of Catalytic Materials. *ACS Catalysis*, **2019**, 9, 2752-2759	13.1	95
239	Origins of optical absorption and emission lines in AlN. *Applied Physics Letters*, **2014**, 105, 111104	3.4	94
238	New perspective on formation energies and energy levels of point defects in nonmetals. *Physical Review Letters*, **2012**, 108, 066404	7.4	93
237	Influence of the core-valence interaction and of the pseudopotential approximation on the electron self-energy in semiconductors. *Physical Review Letters*, **2008**, 101, 106404	7.4	92
236	Clean and As-Covered Zinc-Blende GaN (001) Surfaces: Novel Surface Structures and Surfactant Behavior. *Physical Review Letters*, **1998**, 80, 3097-3100	7.4	92
235	Temperature-Dependent Morphology, Magnetic and Optical Properties of Li-Doped MgO. *ChemCatChem*, **2010**, 2, 854-862	5.2	91
234	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		91

233	Unraveling the stability of polypeptide helices: critical role of van der Waals interactions. *Physical Review Letters*, **2011**, 106, 118102	7.4	90
232	Xe adsorption on metal surfaces: First-principles investigations. *Physical Review B*, **2005**, 72,	3.3	90
231	Hybrid functionals for large periodic systems in an all-electron, numeric atom-centered basis framework. *Computer Physics Communications*, **2015**, 192, 60-69	4.2	89
230	Atomic and electronic structures of GaAs(110) and their alkali-adsorption-induced changes. *Physical Review Letters*, **1991**, 67, 1031-1034	7.4	89
229	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. *Physical Review B*, **2013**, 88,	3.3	88
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226	Electronic properties of lanthanide oxides from the GW perspective. *Physical Review B*, **2012**, 86,	3.3	86
225	Examination of the concept of degree of rate control by first-principles kinetic Monte Carlo simulations. *Surface Science*, **2009**, 603, 1724-1730	1.8	86
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223	Partial dissociation of water on Fe3O4(001): adsorbate induced charge and orbital order. *Physical Review Letters*, **2009**, 103, 176102	7.4	84
222	Insight from first principles into the nature of the bonding between water molecules and 4d metal surfaces. *Journal of Chemical Physics*, **2009**, 130, 184707	3.9	84
221	Exciting prospects for solids: Exact-exchange based functionals meet quasiparticle energy calculations. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 929-945	1.3	82
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218	Alloy catalyst in a reactive environment: the example of ag-cu particles for ethylene epoxidation. *Physical Review Letters*, **2010**, 104, 035503	7.4	80
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216	AB Initio Atomistic Thermodynamics and Statistical Mechanics of Surface Properties and Functions **2005**, 149-194		78

215	Exact-exchange-based quasiparticle energy calculations for the band gap, effective masses, and deformation potentials of ScN. *Physical Review B*, **2006**, 74,	3.3	78
214	The NOMAD laboratory: from data sharing to artificial intelligence. *JPhys Materials*, **2019**, 2, 036001	4.2	77
213	Comparison of the full-potential and frozen-core approximation approaches to density-functional calculations of surfaces. *Physical Review B*, **2006**, 73,	3.3	75
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211	Density-functional theory study of the initial oxygen incorporation in Pd(111). *Physical Review B*, **2005**, 71,	3.3	74
210	Effects of strain on the band structure of group-III nitrides. *Physical Review B*, **2014**, 90,	3.3	73
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208	Surface coordination chemistry: dihydrogen versus hydride complexes on RuO2(110). *Angewandte Chemie - International Edition*, **2003**, 42, 2151-4	16.4	73
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206	Secondary Structure of Ac-Alan-LysH+ Polyalanine Peptides (n = 5,10,15) in Vacuo: Helical or Not?. *Journal of Physical Chemistry Letters*, **2010**, 1, 3465-3470	6.4	72
205	THEORY OF ALKALI-METAL ADSORPTION ON CLOSE-PACKED METAL SURFACES. *Surface Review and Letters*, **1995**, 02, 317-343	1.1	70
204	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	7.4	69
203	Surface Relaxation and Ferromagnetism of Rh(001). *Physical Review Letters*, **1997**, 78, 1299-1302	7.4	69
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201	Density-functional theory study of half-metallic heterostructures: interstitial Mn in Si. *Physical Review Letters*, **2007**, 98, 117202	7.4	68
200	Hubbard correlations and charge transfer at the GaAs(110) surface with alkali adsorbates. *Physical Review Letters*, **1993**, 70, 351-354	7.4	67
199	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	65
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193	Trends in the chemical reactivity of surfaces studied by ab initio quantum-dynamics calculations. *Physical Review B*, **1999**, 59, 13297-13300	3.3	63
192	Stability and metastability of clusters in a reactive atmosphere: theoretical evidence for unexpected stoichiometries of MgMOx. *Physical Review Letters*, **2013**, 111, 135501	7.4	62
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