Matthias Scheffler

List of Publications by Year in Descending Order

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	Learning Design Rules for Selective Oxidation Catalysts from High-Throughput Experimentation and Artificial Intelligence.. *ACS Catalysis*, **2022**, 12, 2223-2232	13.1	5
375	Artificial-intelligence-driven discovery of catalyst genes with application to CO activation on semiconductor oxides.. *Nature Communications*, **2022**, 13, 419	17.4	13
374	SISSO++: A C++ Implementation of the Sure-Independence Screening and Sparsifying Operator Approach. *Journal of Open Source Software*, **2022**, 7, 3960	5.2	1
373	FAIR data enabling new horizons for materials research.. *Nature*, **2022**, 604, 635-642	50.4	6
372	Roadmap on organic–inorganic hybrid perovskite semiconductors and devices. *APL Materials*, **2021**, 9, 109202	5.7	28
371	All-electron periodic G0W0 implementation with numerical atomic orbital basis functions: Algorithm and benchmarks. *Physical Review Materials*, **2021**, 5,	3.2	11
370	OPTIMADE, an API for exchanging materials data. *Scientific Data*, **2021**, 8, 217	8.2	8
369	Materials genes of heterogeneous catalysis from clean experiments and artificial intelligence.. *MRS Bulletin*, **2021**, 46, 1016-1026	3.2	11
368	GIMS: Graphical Interface for Materials Simulations. *Journal of Open Source Software*, **2021**, 6, 2767	5.2	
367	Artificial intelligence for high-throughput discovery of topological insulators: The example of alloyed tetradymites. *Physical Review Materials*, **2020**, 4,	3.2	13
366	Anharmonicity measure for materials. *Physical Review Materials*, **2020**, 4,	3.2	14
365	FHI-vibes: Ab Initio Vibrational Simulations. *Journal of Open Source Software*, **2020**, 5, 2671	5.2	3
364	Big Data-Driven Materials Science and Its FAIR Data Infrastructure **2020**, 49-73		12
363	Pentacene and tetracene molecules and films on H/Si(111): level alignment from hybrid density functional theory. *Electronic Structure*, **2020**, 2, 035002	2.6	6
362	Towards Experimental Handbooks in Catalysis. *Topics in Catalysis*, **2020**, 63, 1683-1699	2.3	11
361	Fully anharmonic nonperturbative theory of vibronically renormalized electronic band structures. *Physical Review B*, **2020**, 102,	3.3	11
360	Identifying domains of applicability of machine learning models for materials science. *Nature Communications*, **2020**, 11, 4428	17.4	29

359	Simultaneous learning of several materials properties from incomplete databases with multi-task SISSO. *JPhys Materials*, **2019**, 2, 024002	4.2	45
358	Modulation of the Work Function by the Atomic Structure of Strong Organic Electron Acceptors on H-Si(111). *Advanced Electronic Materials*, **2019**, 5, 1800891	6.4	21
357	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	10
356	The NOMAD laboratory: from data sharing to artificial intelligence. *JPhys Materials*, **2019**, 2, 036001	4.2	77
355	New tolerance factor to predict the stability of perovskite oxides and halides. *Science Advances*, **2019**, 5, eaav0693	14.3	376
354	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	0.6	7
353	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	6.4	15
352	Determining surface phase diagrams including anharmonic effects. *Physical Review B*, **2019**, 100,	3.3	5
351	Two-to-three dimensional transition in neutral gold clusters: The crucial role of van der Waals interactions and temperature. *Physical Review Materials*, **2019**, 3,	3.2	24
350	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,	3.9	5
349	Big Data-Driven Materials Science and Its FAIR Data Infrastructure **2019**, 1-25		3
348	Beyond Scaling Relations for the Description of Catalytic Materials. *ACS Catalysis*, **2019**, 9, 2752-2759	13.1	95
347	Parametrically constrained geometry relaxations for high-throughput materials science. *Npj Computational Materials*, **2019**, 5,	10.9	8
346	Crowd-sourcing materials-science challenges with the NOMAD 2018 Kaggle competition. *Npj Computational Materials*, **2019**, 5,	10.9	22
345	Compact representation of one-particle wavefunctions and scalar fields obtained from electronic-structure calculations. *Computer Physics Communications*, **2019**, 237, 42-46	4.2	
344	First-principles supercell calculations of small polarons with proper account for long-range polarization effects. *New Journal of Physics*, **2018**, 20, 033023	2.9	25
343	Local Atomic Arrangements and Band Structure of Boron Carbide. *Angewandte Chemie - International Edition*, **2018**, 57, 6130-6135	16.4	25
342	Insightful classification of crystal structures using deep learning. *Nature Communications*, **2018**, 9, 2775	17.4	151

341	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
340	NOMAD: The FAIR concept for big data-driven materials science. *MRS Bulletin*, **2018**, 43, 676-682	3.2	155
339	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	20
338	Performance of various density-functional approximations for cohesive properties of 64 bulk solids. *New Journal of Physics*, **2018**, 20, 063020	2.9	110
337	Lattice dynamics calculations based on density-functional perturbation theory in real space. *Computer Physics Communications*, **2017**, 215, 26-46	4.2	27
336	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
335	Learning physical descriptors for materials science by compressed sensing. *New Journal of Physics*, **2017**, 19, 023017	2.9	72
334	Li/MgO Catalysts Doped with Alio-valent Ions. Part II: Local Topology Unraveled by EPR/NMR and DFT Modeling. *ChemCatChem*, **2017**, 9, 3597-3610	5.2	10
333	Computational materials: Open data settled in materials theory. *Nature*, **2017**, 548, 523	50.4	6
332	Uncovering structure-property relationships of materials by subgroup discovery. *New Journal of Physics*, **2017**, 19, 013031	2.9	61
331	Formation of Vacancies in Si- and Ge-based Clathrates: Role of Electron Localization and Symmetry Breaking. *Physical Review Letters*, **2017**, 118, 236401	7.4	16
330	Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. *Npj Computational Materials*, **2017**, 3,	10.9	53
329	Ab□Initio Green-Kubo Approach for the Thermal Conductivity of Solids. *Physical Review Letters*, **2017** , 118, 175901	7.4	58
328	Towards Efficient Orbital-Dependent Density Functionals for Weak and Strong Correlation. *Physical Review Letters*, **2016**, 117, 133002	7.4	18
327	Density functional theory study of the □phase transition in cerium: Role of electron correlation and f-orbital localization. *Physical Review B*, **2016**, 93,	3.3	15
326	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,	3.3	40
325	Self-consistent Green's function embedding for advanced electronic structure methods based on a dynamical mean-field concept. *Physical Review B*, **2016**, 93,	3.3	26
324	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784

323	Wave-function inspired density functional applied to the H2/${{rm{H}}}_{2}^{+}$ challenge. *New Journal of Physics*, **2016**, 18, 073026	2.9	10
322	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
321	Multiscale approach to the electronic structure of doped semiconductor surfaces. *Physical Review B* , **2015**, 91,	3.3	24
320	Big data of materials science: critical role of the descriptor. *Physical Review Letters*, **2015**, 114, 105503	7.4	495
319	All-electron formalism for total energy strain derivatives and stress tensor components for numeric atom-centered orbitals. *Computer Physics Communications*, **2015**, 190, 33-50	4.2	58
318	Evidence for photogenerated intermediate hole polarons in ZnO. *Nature Communications*, **2015**, 6, 6901	17.4	42
317	Native like helices in a specially designed peptide in the gas phase. *Physical Chemistry Chemical Physics*, **2015**, 17, 5376-85	3.6	13
316	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
315	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, 7373-85	3.6	42
314	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
313	Why graphene growth is very different on the C face than on the Si face of SiC: Insights from surface equilibria and the (3)SiC(1101) reconstruction. *Physical Review B*, **2015**, 91,	3.3	11
312	Beyond the GW approximation: A second-order screened exchange correction. *Physical Review B*, **2015**, 92,	3.3	37
311	Static correlation and electron localization in molecular dimers from the self-consistent RPA and GW approximation. *Physical Review B*, **2015**, 91,	3.3	46
310	Length dependence of ionization potentials of transacetylenes: Internally consistent DFT/GW approach. *Physical Review B*, **2015**, 92,	3.3	25
309	Insight into organic reactions from the direct random phase approximation and its corrections. *Journal of Chemical Physics*, **2015**, 143, 144115	3.9	11
308	Integer versus Fractional Charge Transfer at Metal(/Insulator)/Organic Interfaces: Cu(/NaCl)/TCNE. *ACS Nano*, **2015**, 9, 5391-404	16.7	48
307	Multi-lattice Kinetic Monte Carlo Simulations from First Principles: Reduction of the Pd(100) Surface Oxide by CO. *ACS Catalysis*, **2015**, 5, 1199-1209	13.1	23
306	Validation challenge of density-functional theory for peptides-example of Ac-Phe-Ala5-LysH(+). *Journal of Physical Chemistry A*, **2014**, 118, 7349-59	2.8	38

305	First-principles description of charge transfer in donor-acceptor compounds from self-consistent many-body perturbation theory. *Physical Review B*, **2014**, 90,	3.3	42
304	Effects of strain on the band structure of group-III nitrides. *Physical Review B*, **2014**, 90,	3.3	73
303	Modeling adsorption and reactions of organic molecules at metal surfaces. *Accounts of Chemical Research*, **2014**, 47, 3369-77	24.3	177
302	Efficientab initioschemes for finding thermodynamically stable and metastable atomic structures: benchmark of cascade genetic algorithms. *New Journal of Physics*, **2014**, 16, 123016	2.9	33
301	Origins of optical absorption and emission lines in AlN. *Applied Physics Letters*, **2014**, 105, 111104	3.4	94
300	Ferroelastic switching of doped zirconia: Modeling and understanding from first principles. *Physical Review B*, **2014**, 90,	3.3	20
299	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
298	Thermodynamic equilibrium conditions of graphene films on SiC. *Physical Review Letters*, **2013**, 111, 065502	7.4	32
297	How cations change peptide structure. *Chemistry - A European Journal*, **2013**, 19, 11224-34	4.8	32
296	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
295	Self-consistent GW: All-electron implementation with localized basis functions. *Physical Review B*, **2013**, 88,	3.3	120
294	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
293	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
292	FHI-gap: A code based on the all-electron augmented plane wave method. *Computer Physics Communications*, **2013**, 184, 348-366	4.2	44
291	Space-charge transfer in hybrid inorganic-organic systems. *Physical Review Letters*, **2013**, 111, 226802	7.4	59
290	Hybrid density functional theory meets quasiparticle calculations: A consistent electronic structure approach. *Physical Review B*, **2013**, 88,	3.3	99
289	Impact of vibrational entropy on the stability of unsolvated peptide helices with increasing length. *Journal of Physical Chemistry B*, **2013**, 117, 5574-84	3.4	28
288	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	3.8	7

287	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
286	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	50
285	Interface dipoles of organic molecules on Ag(111) in hybrid density-functional theory. *New Journal of Physics*, **2013**, 15, 123028	2.9	54
284	Concentration of vacancies at metal-oxide surfaces: case study of MgO(100). *Physical Review Letters*, **2013**, 111, 045502	7.4	85
283	Large work function reduction by adsorption of a molecule with a negative electron affinity: pyridine on ZnO(1010). *Journal of Chemical Physics*, **2013**, 139, 174701	3.9	62
282	Numeric atom-centered-orbital basis sets with valence-correlation consistency from H to Ar. *New Journal of Physics*, **2013**, 15, 123033	2.9	65
281	Renormalized second-order perturbation theory for the electron correlation energy: Concept, implementation, and benchmarks. *Physical Review B*, **2013**, 88,	3.3	88
280	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
279	An Introduction to the Theory of Crystalline Elemental Solids and their Surfaces **2013**, 13-72		5
278	Random-phase approximation and its applications in computational chemistry and materials science. *Journal of Materials Science*, **2012**, 47, 7447-7471	4.3	389
277	Strain effects and band parameters in MgO, ZnO, and CdO. *Applied Physics Letters*, **2012**, 101, 152105	3.4	56
276	Electronic properties of lanthanide oxides from the GW perspective. *Physical Review B*, **2012**, 86,	3.3	86
275	Role of nitrogen vacancies in the luminescence of Mg-doped GaN. *Applied Physics Letters*, **2012**, 100, 142110	3.4	107
274	New perspective on formation energies and energy levels of point defects in nonmetals. *Physical Review Letters*, **2012**, 108, 066404	7.4	93
273	Toward Low-Temperature Dehydrogenation Catalysis: Isophorone Adsorbed on Pd(111). *Journal of Physical Chemistry Letters*, **2012**, 3, 582-6	6.4	33
272	Benchmark of GW methods for azabenzenes. *Physical Review B*, **2012**, 86,	3.3	132
271	Benzene adsorbed on metals: Concerted effect of covalency and van der Waals bonding. *Physical Review B*, **2012**, 86,	3.3	227
270	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

269	First-principles optical spectra for F centers in MgO. *Physical Review Letters*, **2012**, 108, 126404	7.4	131
268	Resolution-of-identity approach to Hartree□Fock, hybrid density functionals, RPA, MP2 andGWwith numeric atom-centered orbital basis functions. *New Journal of Physics*, **2012**, 14, 053020	2.9	411
267	Assessment of correlation energies based on the random-phase approximation. *New Journal of Physics*, **2012**, 14, 043002	2.9	111
266	Impact of widely used approximations to theG0W0method: an all-electron perspective. *New Journal of Physics*, **2012**, 14, 023006	2.9	35
265	Benzene adsorbed on Si(001): The role of electron correlation and finite temperature. *Physical Review B*, **2012**, 85,	3.3	27
264	Accurate and efficient method for many-body van der Waals interactions. *Physical Review Letters*, **2012**, 108, 236402	7.4	920
263	Density-functional theory for f-electron systems: the □□phase transition in cerium. *Physical Review Letters*, **2012**, 109, 146402	7.4	51
262	Free gold clusters: beyond the static, monostructure description. *Faraday Discussions*, **2011**, 152, 153-67; discussion 203-25	3.6	32
261	Beyond the random-phase approximation for the electron correlation energy: the importance of single excitations. *Physical Review Letters*, **2011**, 106, 153003	7.4	171
260	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
259	Van der Waals interactions in ionic and semiconductor solids. *Physical Review Letters*, **2011**, 107, 245501	7.4	131
258	Analytic many-body potential for GaAs(001) homoepitaxy: Bulk and surface properties. *Physical Review B*, **2011**, 83,	3.3	16
257	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
256	Aktivierungsenergien f□die Diffusion von Defekten in Silicium: die Rolle des Austauschkorrelationsfunktionals. *Angewandte Chemie*, **2011**, 123, 10403-10407	3.6	
255	Die CO-Oxidation als Modellreaktion f□heterogene Prozesse. *Angewandte Chemie*, **2011**, 123, 10242-10276	3.6	73
254	Activation energies for diffusion of defects in silicon: the role of the exchange-correlation functional. *Angewandte Chemie - International Edition*, **2011**, 50, 10221-5	16.4	29
253	CO oxidation as a prototypical reaction for heterogeneous processes. *Angewandte Chemie - International Edition*, **2011**, 50, 10064-94	16.4	510
252	Hydrogen bonds and van der waals forces in ice at ambient and high pressures. *Physical Review Letters*, **2011**, 107, 185701	7.4	181

251	Enhanced dipole moments in photo-excited TTF□TCNQ dimers. *New Journal of Physics*, **2011**, 13, 073039	2.9	8
250	Unraveling the stability of polypeptide helices: critical role of van der Waals interactions. *Physical Review Letters*, **2011**, 106, 118102	7.4	90
249	Band parameters and strain effects in ZnO and group-III nitrides. *Semiconductor Science and Technology*, **2011**, 26, 014037	1.8	48
248	Stable structure and magnetic state of ultrathin CrAs films on GaAs(001): A density functional theory study. *Physical Review B*, **2010**, 82,	3.3	13
247	Role of strain in polarization switching in semipolar InGaN/GaN quantum wells. *Applied Physics Letters*, **2010**, 97, 181102	3.4	29
246	Coverage-Dependent Adsorption Mode of Water on Fe3O4(001): Insights from First Principles Calculations. *Journal of Physical Chemistry C*, **2010**, 114, 11148-11156	3.8	63
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	First-principles modeling of localized d states with the GW@LDA+U approach. *Physical Review B*, **2010**, 82,	3.3	188
243	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
242	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
241	Van der Waals Interactions Between Organic Adsorbates and at Organic/Inorganic Interfaces. *MRS Bulletin*, **2010**, 35, 435-442	3.2	244
240	First-principles study of the mechanism of ethylene epoxidation over Ag□Cu particles. *Journal of Materials Chemistry*, **2010**, 20, 10521		20
239	Large-scale surface reconstruction energetics of Pt(100) and Au(100) by all-electron density functional theory. *Physical Review B*, **2010**, 82,	3.3	46
238	Electronic band structure of zirconia and hafnia polymorphs from the GW perspective. *Physical Review B*, **2010**, 81,	3.3	157
237	Alloy catalyst in a reactive environment: the example of ag-cu particles for ethylene epoxidation. *Physical Review Letters*, **2010**, 104, 035503	7.4	80
236	Temperature-Dependent Morphology, Magnetic and Optical Properties of Li-Doped MgO. *ChemCatChem*, **2010**, 2, 854-862	5.2	91
235	Exploring the random phase approximation: Application to CO adsorbed on Cu(111). *Physical Review B*, **2009**, 80,	3.3	136
234	Structural stability and magnetic and electronic properties of Co2MnSi(001)/MgO heterostructures: a density-functional theory study. *Physical Review Letters*, **2009**, 103, 046802	7.4	30

233	Partial dissociation of water on Fe3O4(001): adsorbate induced charge and orbital order. *Physical Review Letters*, **2009**, 103, 176102	7.4	84
232	Thermodynamics of the Heusler alloy Co2MnSi: A combined density functional theory and cluster expansion study. *Physical Review B*, **2009**, 79,	3.3	58
231	Dispersion-corrected Møller-Plesset second-order perturbation theory. *Journal of Chemical Physics*, **2009**, 131, 094106	3.9	172
230	Density functional theory study of the conformational space of an infinitely long polypeptide chain. *Journal of Chemical Physics*, **2009**, 131, 085104	3.9	16
229	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
228	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	3.9	57
227	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
226	AgCu alloy surfaces in an oxidizing environment: A first-principles study. *Surface Science*, **2009**, 603, 1467-1475	1.8	35
225	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
224	Ab initio molecular simulations with numeric atom-centered orbitals. *Computer Physics Communications*, **2009**, 180, 2175-2196	4.2	1637
223	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
222	Controlling polarization at insulating surfaces: quasiparticle calculations for molecules adsorbed on insulator films. *Physical Review Letters*, **2009**, 103, 056803	7.4	62
221	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
220	Experimental and theoretical study of oxygen adsorption structures on Ag(111). *Physical Review B*, **2009**, 80,	3.3	80
219	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
218	Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN. *Applied Physics Letters*, **2009**, 95, 121111	3.4	132
217	Two-step mechanism for low-temperature oxidation of vacancies in graphene. *Physical Review Letters*, **2009**, 102, 166104	7.4	106
216	Localized and itinerant states in lanthanide oxides united by GW @ LDA+U. *Physical Review Letters*, **2009**, 102, 126403	7.4	142

215	Compensation Mechanisms and Functionality of Transition Metal Oxide Surfaces and Interfaces: A Density Functional Theory Study **2009**, 709-717		1
214	Sources of electrical conductivity in SnO2. *Physical Review Letters*, **2008**, 101, 055502	7.4	309
213	Exchange interactions and critical temperature of bulk and thin films of MnSi: A density functional theory study. *Physical Review B*, **2008**, 78,	3.3	37
212	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
211	Screening in two dimensions: GW calculations for surfaces and thin films using the repeated-slab approach. *Physical Review B*, **2008**, 77,	3.3	56
210	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
209	Nonadiabatic effects in the dissociation of oxygen molecules at the Al(111) surface. *Physical Review B*, **2008**, 77,	3.3	103
208	First-principles investigation of Ag-Cu alloy surfaces in an oxidizing environment. *Physical Review B*, **2008**, 77,	3.3	40
207	CO oxidation on Pd(100) at technologically relevant pressure conditions: First-principles kinetic Monte Carlo study. *Physical Review B*, **2008**, 77,	3.3	78
206	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
205	How strong is the bond between water and salt?. *Surface Science*, **2008**, 602, L135-L138	1.8	21
204	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
203	CO oxidation at Pd(100): A first-principles constrained thermodynamics study. *Physical Review B*, **2007**, 75,	3.3	106
202	Ab initiostudy of the half-metal to metal transition in strained magnetite. *New Journal of Physics*, **2007**, 9, 5-5	2.9	48
201	Does phenomenological kinetics provide an adequate description of heterogeneous catalytic reactions?. *Journal of Chemical Physics*, **2007**, 126, 204711	3.9	108
200	Dielectric anisotropy in the GW spacetime method. *Computer Physics Communications*, **2007**, 176, 1-13	4.2	43
199	Transition-metal silicides as materials for magnet-semiconductor heterostructuresa). *Journal of Applied Physics*, **2007**, 101, 081725	2.5	13
198	Ultrathin oxides: bulk-oxide-like model surfaces or unique films?. *Physical Review Letters*, **2007**, 99, 086101	7.4	52

197	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
196	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
195	Nonadiabatic potential-energy surfaces by constrained density-functional theory. *Physical Review B*, **2007**, 75,	3.3	75
194	Density-functional theory study of half-metallic heterostructures: interstitial Mn in Si. *Physical Review Letters*, **2007**, 98, 117202	7.4	68
193	Density-functional study of Mn monosilicide on the Si(111) surface: Film formation versus island nucleation. *Physical Review B*, **2007**, 76,	3.3	28
192	Density functional theory study of flat and stepped NaCl(001). *Physical Review B*, **2007**, 76,	3.3	37
191	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
190	Converged properties of clean metal surfaces by all-electron first-principles calculations. *Surface Science*, **2006**, 600, 703-715	1.8	225
189	Behler, Reuter, and Scheffler Reply:. *Physical Review Letters*, **2006**, 96,	7.4	5
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