Catherine Stampfl

List of Publications by Year in Descending Order

256 papers	11,830 citations	57 h-index	100 g-index
272 ext. papers	12,920 ext. citations	4.3 avg, IF	6.67 L-index

#	Paper	IF	Citations
256	Vacancy-Induced Thermal Transport and Tensile Mechanical Behavior of Monolayer Honeycomb BeO.. *ACS Omega*, **2022**, 7, 4525-4537	3.9	2
255	Temperature and interlayer coupling induced thermal transport across graphene/2D-SiC van der Waals heterostructure.. *Scientific Reports*, **2022**, 12, 761	4.9	0
254	Atomic and Molecular Hydrogen Impurities in Hybrid Perovskite Solar Cells. *Journal of Physical Chemistry C*, **2022**, 126, 1721-1728	3.8	0
253	Band-gap engineering, magnetic behavior and Dirac-semimetal character in the MoSi2N4 nanoribbon with armchair and zigzag edges. *Journal Physics D: Applied Physics*, **2022**, 55, 035301	3	7
252	Monoelemental two-dimensional iodinene nanosheets: a first-principles study of the electronic and optical properties. *Journal Physics D: Applied Physics*, **2022**, 55, 135104	3	
251	Deep Neural Skill Assessment and Transfer: Application to Robotic Surgery Training **2021**,		1
250	Twist-Dependent Electron Charge Transfer and Transport in Phosphorene□raphene Heterobilayers. *Journal of Physical Chemistry C*, **2021**, 125, 25886-25897	3.8	
249	Hydrogen-Anion-Induced Carrier Recombination in MAPbI Perovskite Solar Cells. *Journal of Physical Chemistry Letters*, **2021**, 12, 10677-10683	6.4	3
248	Resolving Deactivation Pathways of Co Porphyrin-Based Electrocatalysts for CO2 Reduction in Aqueous Medium. *ACS Catalysis*, **2021**, 11, 3715-3729	13.1	11
247	First-principles investigation of intrinsic point defects in perovskite CsSnBr3. *Physical Review Materials*, **2021**, 5,	3.2	5
246	Semiconducting Chalcogenide Alloys Based on the (Ge, Sn, Pb) (S, Se, Te) Formula with Outstanding Properties: A First-Principles Calculation Study. *ACS Omega*, **2021**, 6, 9433-9441	3.9	9
245	Effect of electric field and vertical strain on the electro-optical properties of the MoSi2N4 bilayer: A first-principles calculation. *Journal of Applied Physics*, **2021**, 129, 155103	2.5	23
244	A Dirac-semimetal two-dimensional BeN4: Thickness-dependent electronic and optical properties. *Applied Physics Letters*, **2021**, 118, 203103	3.4	32
243	Electrode-induced impurities in tin halide perovskite solar cell material CsSnBr3 from first principles. *Npj Computational Materials*, **2021**, 7,	10.9	4
242	Modeling and Experimental Study of the Electron Transfer Kinetics for Non-ideal Electrodes Using Variable-Frequency Square Wave Voltammetry. *Analytical Chemistry*, **2021**, 93, 10175-10186	7.8	2
241	Thermal transport in monolayer zinc-sulfide: effects of length, temperature and vacancy defects. *Nanotechnology*, **2021**, 32,	3.4	2
240	Transition metal-doped tetra-MoN2 monolayers as an electrochemical catalyst for CO2 reduction: A density functional theory study. *Catalysis Communications*, **2021**, 149, 106212	3.2	1

239	Confined Ru Nanocatalysts on Surface to Enhance Ammonia Synthesis: An In situ ETEM Study. *ChemCatChem*, **2021**, 13, 534-538	5.2	3
238	Attenuation of Redox Switching and Rectification in Azulenequinones/Hydroquinones after B and N Doping: A First-Principles Investigation. *Advanced Theory and Simulations*, **2021**, 4, 2000203	3.5	2
237	Morphogenesis of mesoscopic surface patterns formed in polarized two-photon etching of diamond. *Carbon*, **2021**, 173, 271-285	10.4	1
236	Two-dimensional Janus semiconductor BiTeCl and BiTeBr monolayers: a first-principles study on their tunable electronic properties an electric field and mechanical strain. *Physical Chemistry Chemical Physics*, **2021**, 23, 15216-15223	3.6	17
235	Case Report: Utilizing AI and NLP to Assist with Healthcare and Rehabilitation During the COVID-19 Pandemic. *Frontiers in Artificial Intelligence*, **2021**, 4, 613637	3	6
234	Mechanistic studies of oxygen reduction and evolution reactions on Ni3S2 surfaces. *Applied Catalysis A: General*, **2021**, 624, 118324	5.1	2
233	Superior tunable photocatalytic properties for water splitting in two dimensional GeC/SiC van der Waals heterobilayers. *Scientific Reports*, **2021**, 11, 17739	4.9	1
232	Strong tribo-piezoelectric effect in bilayer indium nitride (InN). *Scientific Reports*, **2021**, 11, 18669	4.9	2
231	. *IEEE Access*, **2021**, 9, 116254-116264	3.5	1
230	Band-gap control of graphenelike borocarbonitride gBC6N bilayers by electrical gating. *Physical Review B*, **2020**, 102,	3.3	26
229	Robotics, Smart Wearable Technologies, and Autonomous Intelligent Systems for Healthcare During the COVID-19 Pandemic: An Analysis of the State of the Art and Future Vision. *Advanced Intelligent Systems*, **2020**, 2, 2000071	6	113
228	Role of knock-on in electron beam induced etching of diamond. *Carbon*, **2020**, 164, 51-58	10.4	2
227	First-principles investigation of nonmetal doped single-layer BiOBr as a potential photocatalyst with a low recombination rate. *Physical Chemistry Chemical Physics*, **2020**, 22, 15354-15364	3.6	45
226	Transition metal-doped borophene as potential oxygen and hydrogen evolution electrocatalyst: A density functional theory study. *Catalysis Communications*, **2020**, 144, 106090	3.2	10
225	Modeling and Emulating a Physiotherapist's Role in Robot-Assisted Rehabilitation. *Advanced Intelligent Systems*, **2020**, 2, 1900181	6	9
224	Embedding of atoms into the nanopore sites of the CN and CN porous carbon nitride monolayers with tunable electronic properties. *Physical Chemistry Chemical Physics*, **2020**, 22, 6418-6433	3.6	27
223	Dirac half-metallicity of Thin PdCl Nanosheets: Investigation of the Effects of External Fields, Surface Adsorption and Defect Engineering on the Electronic and Magnetic Properties. *Scientific Reports*, **2020**, 10, 213	4.9	26
222	Strain, electric-field and functionalization induced widely tunable electronic properties in MoS/BC , /C N and /[Formula: see text] van der Waals heterostructures. *Nanotechnology*, **2020**, 31, 295202	3.4	34

221	The Electronic, Optical, and Thermoelectric Properties of Monolayer PbTe and the Tunability of the Electronic Structure by External Fields and Defects. *Physica Status Solidi (B): Basic Research*, **2020**, 257, 2000182	1.3	28
220	A First-Principles Study of C N Nanostructures: Control and Engineering of the Electronic and Magnetic Properties of Nanosheets, Tubes and Ribbons. *ChemPhysChem*, **2020**, 21, 164-174	3.2	30
219	High mobility in phosphorene isostructures with low deformation potential. *Physical Chemistry Chemical Physics*, **2020**, 22, 2276-2282	3.6	5
218	Control of CN and CN carbon nitride nanosheets electronic and magnetic properties through embedded atoms. *Physical Chemistry Chemical Physics*, **2020**, 22, 2249-2261	3.6	32
217	Formulation of Multicomponent Lattice Gas Model Cluster Expansions Parameterized on Ab Initio Data: An Introduction to the Ab Initio Mean-Field Augmented Lattice Gas Modeling Code. *Journal of Physical Chemistry C*, **2020**, 124, 2923-2938	3.8	4
216	Tunable electronic properties of the dynamically stable layered mineral PtHgSe (Jacutingaite). *Physical Chemistry Chemical Physics*, **2020**, 22, 24471-24479	3.6	14
215	Oxygen Vacancies in the Single Layer of Ti2CO2 MXene: Effects of Gating Voltage, Mechanical Strain, and Atomic Impurities. *Physica Status Solidi (B): Basic Research*, **2020**, 257, 2000343	1.3	14
214	Exceptional in-plane and interfacial thermal transport in graphene/2D-SiC van der Waals heterostructures. *Scientific Reports*, **2020**, 10, 22050	4.9	10
213	Composition-structure-function correlation of Ca/Zn/AlOx catalysts for the ketonization of acetic acid. *Catalysis Today*, **2020**, 351, 58-67	5.3	11
212	NMR Spectroscopic Characterization of Flame-Made Amorphous Silica-Alumina for Cyclohexanol and Glyceraldehyde Conversion. *ChemCatChem*, **2020**, 12, 287-293	5.2	5
211	A first-principles study of the effects of atom impurities, defects, strain, electric field and layer thickness on the electronic and magnetic properties of the C2N nanosheet. *Carbon*, **2020**, 157, 371-384	10.4	81
210	Cooperation of Ni and CaO at Interface for CO2 Reforming of CH4: A Combined Theoretical and Experimental Study. *ACS Catalysis*, **2019**, 9, 10060-10069	13.1	35
209	Negative Poisson ratio in 2D life-boat structured crystals. *Nanoscale Advances*, **2019**, 1, 1117-1123	5.1	7
208	Non-dissociative adsorption of glycerol on the (111) surface of Ni and Pt-based metallic systems: Hints on reforming activity from d-band center. *Molecular Catalysis*, **2019**, 474, 110412	3.3	2
207	Polymorphic expressions of ultrathin oxidic layers of Mo on Au(111). *Nanoscale*, **2019**, 11, 6023-6035	7.7	5
206	First-principles prediction of phonon-mediated superconductivity in XBC (X = Mg, Ca, Sr, Ba). *Physical Chemistry Chemical Physics*, **2019**, 21, 8767-8773	3.6	5
205	Stability and band offsets between GaAs semiconductor and CeO2 gate dielectric. *AIP Advances*, **2019**, 9, 025117	1.5	2
204	Unravelling the effects of layered supports on Ru nanoparticles for enhancing N2 reduction in photocatalytic ammonia synthesis. *Applied Catalysis B: Environmental*, **2019**, 259, 118026	21.8	22

203	Structural stability and band alignment in the c-plane ZnO/GaN heterostructure. *Semiconductor Science and Technology*, **2019**, 34, 095008	1.8	0
202	Electronic transport investigation of redox-switching of azulenequinones/hydroquinones via first-principles studies. *Physical Chemistry Chemical Physics*, **2019**, 21, 17859-17867	3.6	2
201	Exploiting the Novel Electronic and Magnetic Structure of C3N via Functionalization and Conformation. *Advanced Electronic Materials*, **2019**, 5, 1900459	6.4	33
200	Catalytic arene alkylation over H-Beta zeolite: Influence of zeolite shape selectivity and reactant nucleophilicity. *Journal of Catalysis*, **2019**, 380, 9-20	7.3	11
199	Boron-Doped g-C6N6 Layer as a Metal-Free Photoelectrocatalyst for N2 Reduction Reaction. *Journal of Physical Chemistry C*, **2019**, 123, 28739-28743	3.8	17
198	Strongly enhanced acidity and activity of amorphous silica□lumina by formation of pentacoordinated AlV species. *Journal of Catalysis*, **2019**, 372, 1-7	7.3	19
197	Metal-bipyridine complexes as electrocatalysts for the reduction of CO: a density functional theory study. *Physical Chemistry Chemical Physics*, **2019**, 21, 23742-23748	3.6	5
196	Active sites and mechanism of the direct conversion of methane and carbon dioxide to acetic acid over the zinc-modified H-ZSM-5 zeolite. *Catalysis Science and Technology*, **2019**, 9, 6297-6307	5.5	15
195	Photochemical Etching of Carbonyl Groups from a Carbon Matrix: The (001) Diamond Surface. *Physical Review Letters*, **2019**, 122, 016802	7.4	3
194	Strain-Engineered Ultrahigh Mobility in Phosphorene for Terahertz Transistors. *Advanced Electronic Materials*, **2019**, 5, 1800797	6.4	12
193	Efficient Prediction of Structural and Electronic Properties of Hybrid 2D Materials Using Complementary DFT and Machine Learning Approaches. *Advanced Theory and Simulations*, **2019**, 2, 1800128	3.5	34
192	Band alignment of nonpolar (101□0) ZnO on (112) LaAlO3. *Solid State Communications*, **2019**, 287, 23-26	1.6	3
191	Identification of Vicinal Silanols and Promotion of Their Formation on MCM-41 via Ultrasonic Assisted One-Step Room-Temperature Synthesis for Beckmann Rearrangement. *Industrial & Engineering Chemistry Research*, **2018**, 57, 5550-5557	3.9	12
190	Stability and band offsets of nonpolar (112□0) ZnO on (001) LaAlO 3. *Vacuum*, **2018**, 150, 29-34	3.7	10
189	Magnetic properties of stoichiometric and defective CoS. *Physical Chemistry Chemical Physics*, **2018**, 20, 2356-2362	3.6	11
188	Stability and band offsets between c-plane ZnO semiconductor and LaAlO3 gate dielectric. *Journal of Applied Physics*, **2018**, 123, 115302	2.5	2
187	Effect of an Al-adlayer in the c-plane ZnO/AlN heterostructure. *Europhysics Letters*, **2018**, 122, 26003	1.6	1
186	The role of vacancies in electric field mediated graphene oxide reduction. *Applied Physics Letters*, **2018**, 113, 073103	3.4	1

185	Predicting the Electric Field Effect on the Lateral Interactions Between Adsorbates: O/Fe(100) from First Principles. *Topics in Catalysis*, **2018**, 61, 763-775	2.3	9
184	Mechanical properties of zirconia, doped and undoped yttria-stabilized cubic zirconia from first-principles. *Journal of Physics and Chemistry of Solids*, **2018**, 122, 51-71	3.9	25
183	Confinement Impact for the Dynamics of Supported Metal Nanocatalyst. *Small*, **2018**, 14, e1801586	11	3
182	Evaluation of van der Waals density functionals for layered materials. *Physical Review Materials*, **2018**, 2,	3.2	47
181	Machine learning the band gap properties of kesterite I2□IV□4 quaternary compounds for photovoltaics applications. *Physical Review Materials*, **2018**, 2,	3.2	21
180	Acidity enhanced [Al]MCM-41 via ultrasonic irradiation for the Beckmann rearrangement of cyclohexanone oxime to e-caprolactam. *Journal of Catalysis*, **2018**, 358, 71-79	7.3	23
179	van der Waals Forces Control the Internal Chemical Structure of Monolayers within the Lamellar Materials CuInP2S6 and CuBiP2Se6. *Journal of Physical Chemistry C*, **2018**, 122, 22675-22687	3.8	11
178	Superconductivity in intercalated buckled two-dimensional materials: KGe. *Physical Chemistry Chemical Physics*, **2018**, 20, 24027-24032	3.6	1
177	First-principles design of bifunctional oxygen reduction and evolution catalysts through bimetallic centers in metal□organic frameworks. *Catalysis Science and Technology*, **2018**, 8, 3666-3674	5.5	13
176	Acceptor doping in the proton conductor SrZrO. *Physical Chemistry Chemical Physics*, **2017**, 19, 11485-11491	3.6	13
175	Near-Perfect Spin Filtering and Negative Differential Resistance in an Fe(II)S Complex. *Journal of Physical Chemistry Letters*, **2017**, 8, 2189-2194	6.4	9
174	Uncovering the Thermo-Kinetic Origins of Phase Ordering in Mixed-Valence Antimony Tetroxide by First-Principles Modeling. *Inorganic Chemistry*, **2017**, 56, 6545-6550	5.1	1
173	Stability and band offsets between Si and LaAlO3. *European Physical Journal B*, **2017**, 90, 1	1.2	2
172	Band offsets in La2O3/InN heterostructures. *Solid State Communications*, **2017**, 265, 19-22	1.6	
171	First-principles investigation of quantum emission from hBN defects. *Nanoscale*, **2017**, 9, 13575-13582	7.7	122
170	Hydrogen Adsorption on Nearly Zigzag-Edged Nanoribbons: A Density Functional Theory Study. *Scientific Reports*, **2017**, 7, 15727	4.9	23
169	TDDFT Study of the Optical Excitation of Nucleic Acid Bases-C Complexes. *Journal of Physical Chemistry A*, **2017**, 121, 9058-9063	2.8	1
168	Benzylation of Arenes with Benzyl Chloride over H-Beta Zeolite: Effects from Acidity and Shape-Selectivity. *Journal of Physical Chemistry C*, **2017**, 121, 15248-15255	3.8	13

167	Detection of adsorbed transition-metal porphyrins by spin-dependent conductance of graphene nanoribbon. *RSC Advances*, **2017**, 7, 29112-29121	3.7	5
166	Mechanism for strong magnetoelectric coupling in dilute magnetic ferroelectrics. *Physical Review B*, **2016**, 94,	3.3	7
165	Multiferroic crossover in perovskite oxides. *Physical Review B*, **2016**, 93,	3.3	26
164	Large spin-filtering effect in Ti-doped defective zigzag graphene nanoribbon. *Physical Chemistry Chemical Physics*, **2016**, 18, 16224-8	3.6	5
163	Enhanced oscillatory rectification and negative differential resistance in pentamantane diamondoid-cumulene systems. *Nanoscale*, **2016**, 8, 3461-6	7.7	6
162	Unraveling the origins of conduction band valley degeneracies in Mg2Si(1-x)Sn(x) thermoelectrics. *Physical Chemistry Chemical Physics*, **2016**, 18, 939-46	3.6	6
161	Endohedral metallofullerenes, M@C60 (M = Ca, Na, Sr): selective adsorption and sensing of open-shell NOx gases. *Physical Chemistry Chemical Physics*, **2016**, 18, 21315-21	3.6	5
160	Communication: Electrical rectification of C59N: The role of anchoring and doping sites. *Journal of Chemical Physics*, **2016**, 144, 021101	3.9	3
159	Br□sted acid sites based on penta-coordinated aluminum species. *Nature Communications*, **2016**, 7, 13820	17.4	73
158	Sensing sulfur-containing gases using titanium and tin decorated zigzag graphene nanoribbons from first-principles. *Physical Chemistry Chemical Physics*, **2015**, 17, 6925-32	3.6	46
157	Molecular adsorption and methanol synthesis on the oxidized Cu/ZnO(0001) surface. *Surface Science*, **2015**, 641, 97-104	1.8	5
156	High On/Off Conductance Switching Ratio via H-Tautomerization in Quinone. *Journal of Chemical Theory and Computation*, **2015**, 11, 4154-8	6.4	12
155	Insights into the Electronic Structure of the Oxygen Species Active in Alkene Epoxidation on Silver. *ACS Catalysis*, **2015**, 5, 5846-5850	13.1	59
154	Structural and electronic properties of SrZrO3 and Sr(Ti,Zr)O3 alloys. *Physical Review B*, **2015**, 92,	3.3	18
153	Bistable Magnetism and Potential for Voltage-Induced Spin Crossover in Dilute Magnetic Ferroelectrics. *Physical Review Letters*, **2015**, 114, 247601	7.4	15
152	Thermodynamic and spectroscopic properties of oxygen on silver under an oxygen atmosphere. *Physical Chemistry Chemical Physics*, **2015**, 17, 9288-312	3.6	70
151	Multiple CO2 capture in stable metal-doped graphene: a theoretical trend study. *RSC Advances*, **2015**, 5, 50975-50982	3.7	33
150	Density-functional prediction of a surface magnetic phase in SrTiO(3)/LaAlO(3) heterostructures induced by Al vacancies. *Physical Review Letters*, **2014**, 113, 186401	7.4	25

149	Adsorbate induced vacancy formation on silver surfaces. *Physical Chemistry Chemical Physics*, **2014**, 16, 9002-14	3.6	16
148	Re-visiting the O/Cu(111) system--when metastable surface oxides could become an issue!. *Physical Chemistry Chemical Physics*, **2014**, 16, 26735-40	3.6	14
147	Real Time Determination of the Electronic Structure of Unstable Reaction Intermediates during Au2O3 Reduction. *Journal of Physical Chemistry Letters*, **2014**, 5, 80-4	6.4	26
146	Electronic and vibrational properties of yttria-stabilised zirconia from first-principles for 10–40mol% Y2O3. *Journal of Physics and Chemistry of Solids*, **2014**, 75, 1252-1264	3.9	9
145	CHx adsorption (x = 1–4) and thermodynamic stability on the CeO2(111) surface: a first-principles investigation. *RSC Advances*, **2014**, 4, 12245	3.7	13
144	Investigation of the vibrational properties of cubic yttria-stabilized zirconia: A combined experimental and theoretical study. *Journal of Physics and Chemistry of Solids*, **2014**, 75, 351-357	3.9	10
143	Stacking-dependent energetics and electronic structure of ultrathin polymorphic V2VI3 topological insulator nanofilms. *Physical Review B*, **2014**, 90,	3.3	8
142	Hybrid functional calculations of point defects and hydrogen in SrZrO3. *Physical Review B*, **2014**, 89,	3.3	34
141	A medium-energy photoemission and ab-initio investigation of cubic yttria-stabilised zirconia. *Journal of Applied Physics*, **2014**, 115, 143502	2.5	4
140	Mitigation of CO poisoning on functionalized Pt-TiN surfaces. *Physical Chemistry Chemical Physics*, **2013**, 15, 19450-6	3.6	23
139	Hydrogen adsorption capacity of adatoms on double carbon vacancies of graphene: A trend study from first principles. *Physical Review B*, **2013**, 87,	3.3	85
138	Early transition metal dopants in cuprous oxide: To spin or not to spin. *Current Applied Physics*, **2013** , 13, 1707-1712	2.6	6
137	Relativity and the nobility of gold. *Materials Chemistry and Physics*, **2013**, 141, 14-17	4.4	9
136	Microscopic origin of n-type behavior in Si-doped AlN. *Physical Review B*, **2013**, 88,	3.3	15
135	Graphene based dots and antidots: a comparative study from first principles. *Journal of Nanoscience and Nanotechnology*, **2013**, 13, 1251-5	1.3	1
134	Vacancies in GaN bulk and nanowires: effect of self-interaction corrections. *Journal of Physics Condensed Matter*, **2012**, 24, 255801	1.8	8
133	Environment-dependent nanomorphology of TiN: the influence of surface vacancies. *Nanoscale*, **2012**, 4, 5183-8	7.7	25
132	Playing with dimensions: rational design for heteroepitaxial p-n junctions. *Nano Letters*, **2012**, 12, 68-76	11.5	26

131	Structure and stability of transition metal nitride interfaces from first-principles: AlN/VN, AlN/TiN, and VN/TiN. *Applied Surface Science*, **2012**, 258, 5638-5645	6.7	32
130	First principles study of 3d transition metal doped . *Journal of Magnetism and Magnetic Materials*, **2012**, 324, 3138-3143	2.8	36
129	The role of titanium nitride supports for single-atom platinum-based catalysts in fuel cell technology. *Physical Chemistry Chemical Physics*, **2012**, 14, 16552-7	3.6	75
128	Band offsets and polarization effects in wurtzite ZnO/Mg0.25Zn0.75O superlattices from first principles. *Physical Review B*, **2012**, 86,	3.3	13
127	A first-principles study of ultrathin nanofilms of MgO-supported TiN. *Physical Chemistry Chemical Physics*, **2012**, 14, 2462-7	3.6	18
126	Hardness analysis of cubic metal mononitrides from first principles. *Physical Review B*, **2012**, 85,	3.3	63
125	Magnetism of Co-doped ZnO epitaxially grown on a ZnO substrate. *Physical Review B*, **2012**, 85,	3.3	49
124	Built-in electric fields and valence band offsets in InN/GaN(0001) superlattices: First-principles investigations. *Journal of Applied Physics*, **2011**, 109, 083721	2.5	33
123	Surface Chemistry and Catalysis from Ab Initio-Based Multiscale Approaches **2011**, 561-588		
122	Design of shallow acceptors in ZnO through early transition metals codoped with N acceptors. *Physical Review B*, **2011**, 83,	3.3	24
121	Magic numbers of nanoholes in graphene: Tunable magnetism and semiconductivity. *Physical Review B*, **2011**, 84,	3.3	35
120	Quantification of graphene based core/shell quantum dots from first principles. *Applied Physics Letters*, **2011**, 99, 183102	3.4	4
119	Cu/ZnO(0001) under oxidating and reducing conditions: A first-principles survey of surface structures. *Physical Review B*, **2011**, 84,	3.3	28
118	Comparison of hydrogen and deuterium adsorption on Pd(100). *Journal of Chemical Physics*, **2010**, 132, 024714	3.9	17
117	Predicting order-disorder phase transitions of O/Pd(111) from ab initio Wang-Landau Monte Carlo calculations. *Physical Review B*, **2010**, 81,	3.3	15
116	Oxygen adsorption on the (1□1) and (2□1) reconstructed C(111) surfaces: a density functional theory study. *Journal of Physics Condensed Matter*, **2010**, 22, 265007	1.8	27
115	Interaction of diamond (111)-(1 □1) and (2 □1) surfaces with OH: a first principles study. *Journal of Physics Condensed Matter*, **2010**, 22, 475005	1.8	8
114	Density functional study of oxygen on Cu(100) and Cu(110) surfaces. *Physical Review B*, **2010**, 81,	3.3	118

113	Band gap engineering of wurtzite and zinc-blende GaN/AlN superlattices from first principles. *Journal of Applied Physics*, **2010**, 108, 103701	2.5	35
112	Coverage and charge-state dependent adsorption of carbon monoxide on the zinc oxide (0001) surface. *Physical Review B*, **2010**, 82,	3.3	13
111	Continuously tunable band gap in GaN/AlN (0001) superlattices via built-in electric field. *Physical Review B*, **2010**, 81,	3.3	22
110	First-principles study of the mechanism of ethylene epoxidation over Ag□u particles. *Journal of Materials Chemistry*, **2010**, 20, 10521		20
109	Alloy catalyst in a reactive environment: the example of ag-cu particles for ethylene epoxidation. *Physical Review Letters*, **2010**, 104, 035503	7.4	80
108	Tunnel magnetoresistance in trilayer junctions from first principles: Cr □layer doped GaN/AlN/GaN (0 0 0 1). *Journal of Magnetism and Magnetic Materials*, **2010**, 322, 395-399	2.8	
107	Reaction intermediates of methanol synthesis and the water□as-shift reaction on the ZnO(0001) surface. *Surface Science*, **2010**, 604, 1742-1751	1.8	28
106	Adsorption of 2-chlorophenol on Cu2O(111)□CuCUS: A first-principles density functional study. *Applied Surface Science*, **2010**, 256, 4764-4770	6.7	6
105	Native defect-induced multifarious magnetism in nonstoichiometric cuprous oxide: First-principles study of bulk and surface properties of Cu2□. *Physical Review B*, **2009**, 79,	3.3	96
104	Vacancies and interstitials in indium nitride: Vacancy clustering and molecular bondlike formation from first principles. *Physical Review B*, **2009**, 79,	3.3	32
103	First-principles investigation of Mn □layer doped GaN/AlN/GaN (0001) tunneling junctions. *Journal of Applied Physics*, **2009**, 106, 043711	2.5	2
102	A first-principles density functional study of chlorophenol adsorption on Cu2O(110):CuO. *Journal of Chemical Physics*, **2009**, 130, 184505	3.9	25
101	Magnetoresistivity model and ionization-energy approximation for ferromagnets. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 1060-1071	1.3	15
100	Ag□u alloy surfaces in an oxidizing environment: A first-principles study. *Surface Science*, **2009**, 603, 1467-1475	1.8	35
99	Ab initio lattice dynamics and thermal expansion of Cu2O. *Physical Review B*, **2009**, 80,	3.3	39
98	Quantum confinement effects in gallium nitride nanostructures: ab initio investigations. *Nanotechnology*, **2009**, 20, 425401	3.4	13
97	Water adsorption on the stoichiometric and reduced CeO2(111) surface: a first-principles investigation. *Physical Chemistry Chemical Physics*, **2009**, 11, 9188-99	3.6	198
96	Atomic and electronic structure of single and multiple vacancies in GaN nanowires from first-principles. *Physical Review B*, **2009**, 79,	3.3	28

95	Defect complexes and cluster doping of InN: First-principles investigations. *Physical Review B*, **2009**, 79,	3.3	33
94	Stability and morphology of cerium oxide surfaces in an oxidizing environment: A first-principles investigation. *Journal of Chemical Physics*, **2009**, 131, 104701	3.9	129
93	Codoping of aluminum and gallium with nitrogen in ZnO: A comparative first-principles investigation. *Physical Review B*, **2009**, 79,	3.3	58
92	Bridging the temperature and pressure gaps: close-packed transition metal surfaces in an oxygen environment. *Journal of Physics Condensed Matter*, **2008**, 20, 184021	1.8	22
91	Trends in adsorption of noble gases He, Ne, Ar, Kr, and Xe on Pd(111)(3□)R30□ All-electron density-functional calculations. *Physical Review B*, **2008**, 77,	3.3	50
90	Nitrogen vacancies in InN: Vacancy clustering and metallic bonding from first principles. *Physical Review B*, **2008**, 77,	3.3	40
89	Morphology of copper nanoparticles in a nitrogen atmosphere: A first-principles investigation. *Physical Review B*, **2008**, 77,	3.3	36
88	Stability, structure, and electronic properties of chemisorbed oxygen and thin surface oxides on Ir(111). *Physical Review B*, **2008**, 78,	3.3	42
87	First-principles investigation of Ag-Cu alloy surfaces in an oxidizing environment. *Physical Review B*, **2008**, 77,	3.3	40
86	Geometry and diameter dependence of the electronic and physical properties of GaN nanowires from first principles. *Physical Review B*, **2008**, 77,	3.3	77
85	Built-in electric field assisted spin injection in Cr and Mn □layer doped AlN/GaN(0001) heterostructures from first principles. *Physical Review B*, **2008**, 78,	3.3	12
84	Shape and surface structure of gold nanoparticles under oxidizing conditions. *Physical Review B*, **2008**, 77,	3.3	46
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