W Gero Schmidt

List of Publications by Year in Descending Order

287 papers	7,341 citations	47 h-index	71 g-index
300 ext. papers	8,032 ext. citations	4.2 avg, IF	6.04 L-index

#	Paper	IF	Citations
287	Reconstructions of the As-Terminated GaAs(001) Surface Exposed to Atomic Hydrogen.. *ACS Omega*, **2022**, 7, 5064-5068	3.9	1
286	Electron Polarons in Lithium Niobate: Charge Localization, Lattice Deformation, and Optical Response. *Crystals*, **2021**, 11, 542	2.3	2
285	Controlled growth of ordered monolayers of N-heterocyclic carbenes on silicon. *Nature Chemistry*, **2021**, 13, 828-835	17.6	12
284	Band Alignment at Ga x In1 P/Al y In1 P Alloy Interfaces from Hybrid Density Functional Theory Calculations. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2000463	1.3	2
283	InP and AlInP(001)(2 4) Surface Oxidation from Density Functional Theory. *ACS Omega*, **2021**, 6, 6297-6304	3.9	3
282	Spin Polarization, Electron-Phonon Coupling, and Zero-Phonon Line of the NV Center in 3-SiC. *Nano Letters*, **2021**, 21, 8119-8125	11.5	4
281	Electronic structure of the Si(111)3R30? surface from theory and photoemission spectroscopy. *Physical Review B*, **2021**, 103,	3.3	4
280	Adatom mediated adsorption of N-heterocyclic carbenes on Cu(111) and Au(111).. *Journal of Computational Chemistry*, **2021**,	3.5	2
279	A photoredox catalysed Heck reaction hole transfer from a Ru(ii)-bis(terpyridine) complex to graphene oxide.. *RSC Advances*, **2020**, 10, 42930-42937	3.7	3
278	Photochemical Ring Opening of Oxirane Modeled by Constrained Density Functional Theory. *ACS Omega*, **2020**, 5, 24057-24063	3.9	2
277	Photocatalytic properties of graphene-supported titania clusters from density-functional theory. *Journal of Computational Chemistry*, **2020**, 41, 1921-1930	3.5	6
276	Toward Efficient Toxic-Gas Detectors: Exploring Molecular Interactions of Sarin and Dimethyl Methylphosphonate with Metal-Centered Phthalocyanine Structures. *Journal of Physical Chemistry C*, **2020**, 124, 6090-6102	3.8	8
275	Vibrational Raman spectroscopy on adsorbate-induced low-dimensional surface structures. *Surface Science Reports*, **2020**, 75, 100480	12.9	0
274	Electron paramagnetic resonance study of ferroelectric phase transition and dynamic effects in a Mn doped [NH][Zn(HCOO)] hybrid formate framework. *Physical Chemistry Chemical Physics*, **2020**, 22, 8513-8521	3.6	1
273	Vibration-Driven Self-Doping of Dangling-Bond Wires on Si(553)-Au Surfaces. *Physical Review Letters*, **2020**, 124, 146802	7.4	6
272	Spin decontamination for magnetic dipolar coupling calculations: Application to high-spin molecules and solid-state spin qubits. *Physical Review Research*, **2020**, 2,	3.9	3
271	Free and defect-bound (bi)polarons in LiNbO3: Atomic structure and spectroscopic signatures from ab initio calculations. *Physical Review Research*, **2020**, 2,	3.9	5

270	Tetracene Ultrathin Film Growth on Hydrogen-Passivated Silicon. *Langmuir*, **2020**, 36, 9099-9113	4	4
269	Subcycle Wannier-Stark Localization by Mid-Infrared Bias in Gallium Arsenide. *EPJ Web of Conferences*, **2019**, 205, 05001	0.3	
268	Accurate and Efficient Spin-Spin Zero-Field Splitting Calculations for Extended Periodic Systems **2019**, 131-140		
267	Excited-state band mapping and momentum-resolved ultrafast population dynamics in In/Si(111) nanowires investigated with XUV-based time- and angle-resolved photoemission spectroscopy. *Physical Review B*, **2019**, 99,	3.3	11
266	Oxygen and potassium vacancies in KTP calculated from first principles. *Journal of Physics Condensed Matter*, **2019**, 31, 385401	1.8	2
265	Potassium titanyl phosphate (KTP) quasiparticle energies and optical response. *JPhys Materials*, **2019**, 2, 045003	4.2	2
264	Quasiparticle and excitonic effects in the optical response of KNbO3. *Physical Review Materials*, **2019**, 3,	3.2	7
263	Water Splitting Reaction at Polar Lithium Niobate Surfaces. *ACS Omega*, **2019**, 4, 3850-3859	3.9	11
262	Electric Field Induced Raman Scattering at the Sb□hP(110) Interface: The Surface Dipole Contribution. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800314	1.3	3
261	Photo-Excited Surface Dynamics from Massively Parallel Constrained-DFT Calculations **2018**, 157-168		
260	Identifying On-Surface Site-Selective Chemical Conversions by Theory-Aided NEXAFS Spectroscopy: The Case of Free-Base Corroles on Ag(111). *Chemistry - A European Journal*, **2018**, 24, 6787-6797	4.8	7
259	Probing quasi-one-dimensional band structures by plasmon spectroscopy. *Physical Review B*, **2018**, 97,	3.3	13
258	Structural dynamics upon photoexcitation-induced charge transfer in a dicopper(i)-disulfide complex. *Physical Chemistry Chemical Physics*, **2018**, 20, 6274-6286	3.6	11
257	Vibrational properties of the Au-(3□)/Si(111) surface reconstruction. *Physical Review B*, **2018**, 97,	3.3	8
256	Calculation of spin-spin zero-field splitting within periodic boundary conditions: Towards all-electron accuracy. *Physical Review B*, **2018**, 97,	3.3	14
255	Temperature stabilizes rough Au/Ge(001) surface reconstructions. *Surface Science*, **2018**, 667, 101-104	1.8	5
254	Signatures of transient Wannier-Stark localization in bulk gallium arsenide. *Nature Communications*, **2018**, 9, 2890	17.4	20
253	Plasmon spectroscopy: Robust metallicity of Au wires on Si(557) upon oxidation. *Physical Review Materials*, **2018**, 2,	3.2	9

252	Imaging of 180? ferroelectric domain walls in uniaxial ferroelectrics by confocal Raman spectroscopy: Unraveling the contrast mechanism. *Physical Review Materials*, **2018**, 2,	3.2	15
251	Impact of finite-temperature and condensed-phase effects on theoretical X-ray absorption spectra of transition metal complexes. *Journal of Computational Chemistry*, **2018**, 40, 712	3.5	4
250	New pyridinium based ionic dyes for the hydrogen evolution reaction. *Tetrahedron*, **2018**, 74, 142-149	2.4	16
249	Polytypism driven zero-field splitting of silicon vacancies in 6H-SiC. *Physical Review B*, **2018**, 98,	3.3	12
248	Beyond the molecular movie: Dynamics of bands and bonds during a photoinduced phase transition. *Science*, **2018**, 362, 821-825	33.3	50
247	Unraveling the Oxidation and Spin State of Mn-Corrole through X-ray Spectroscopy and Quantum Chemical Analysis. *Journal of Physical Chemistry Letters*, **2018**, 9, 6412-6420	6.4	9
246	Spin pairing versus spin chains at Si(553)-Au surfaces. *Physical Review B*, **2018**, 98,	3.3	11
245	Molecular Orbital Rule for Quantum Interference in Weakly Coupled Dimers: Low-Energy Giant Conductivity Switching Induced by Orbital Level Crossing. *Journal of Physical Chemistry Letters*, **2017**, 8, 727-732	6.4	16
244	On-Surface Site-Selective Cyclization of Corrole Radicals. *ACS Nano*, **2017**, 11, 3383-3391	16.7	20
243	Tuning the conductivity along atomic chains by selective chemisorption. *Physical Review B*, **2017**, 95,	3.3	19
242	[Cu (NGuaS)] and its oxidized and reduced derivatives: Confining electrons on a torus. *Journal of Computational Chemistry*, **2017**, 38, 1752-1761	3.5	1
241	Current density analysis of electron transport through molecular wires in open quantum systems. *Journal of Computational Chemistry*, **2017**, 38, 1685-1692	3.5	18
240	Zn-VI quasiparticle gaps and optical spectra from many-body calculations. *Journal of Physics Condensed Matter*, **2017**, 29, 215702	1.8	4
239	Optically excited structural transition in atomic wires on surfaces at the quantum limit. *Nature*, **2017**, 544, 207-211	50.4	77
238	X-ray Spectroscopy of Thin Film Free-Base Corroles: A Combined Theoretical and Experimental Characterization. *Journal of Physical Chemistry C*, **2017**, 121, 2192-2200	3.8	12
237	Electron paramagnetic resonance calculations for hydrogenated Si surfaces. *Physical Review B*, **2017**, 95,	3.3	4
236	Consistent Atomic Geometries and Electronic Structure of Five Phases of Potassium Niobate from Density-Functional Theory. *Advances in Materials Science and Engineering*, **2017**, 2017, 1-13	1.5	11
235	LiNbO surfaces from a microscopic perspective. *Journal of Physics Condensed Matter*, **2017**, 29, 413001	1.8	39

234	Efficient PAW-based bond strength analysis for understanding the In/Si(111)(8 □2) - (4 □1) phase transition. *Journal of Computational Chemistry*, **2017**, 38, 2276-2282	3.5	9
233	Understanding band alignments in semiconductor heterostructures: Composition dependence and type-I□type-II transition of natural band offsets in nonpolar zinc-blende AlxGa1□N/AlyGa1□N composites. *Physical Review B*, **2017**, 95,	3.3	14
232	Solving the Bethe-Salpeter equation for the second-harmonic generation in Zn chalcogenides. *Physical Review B*, **2017**, 96,	3.3	4
231	Optical properties of titanium-doped lithium niobate from time-dependent density-functional theory. *Physical Review Materials*, **2017**, 1,	3.2	6
230	Polaron optical absorption in congruent lithium niobate from time-dependent density-functional theory. *Physical Review Materials*, **2017**, 1,	3.2	7
229	Si(775)-Au atomic chains: Geometry, optical properties, and spin order. *Physical Review Materials*, **2017**, 1,	3.2	12
228	Surface induced vibrational modes in the fluorescence spectra of PTCDA adsorbed on the KCl(100) and NaCl(100) surfaces. *Physical Chemistry Chemical Physics*, **2016**, 18, 32891-32902	3.6	5
227	Atomic size effects studied by transport in single silicide nanowires. *Physical Review B*, **2016**, 93,	3.3	10
226	Vibrational properties of LiNb1□TaxO3 mixed crystals. *Physical Review B*, **2016**, 93,	3.3	15
225	Rare-earth silicide thin films on the Si(111) surface. *Physical Review B*, **2016**, 93,	3.3	25
224	Grand canonical Peierls transition in In/Si(111). *Physical Review B*, **2016**, 93,	3.3	18
223	LiNbO3 electronic structure: Many-body interactions, spin-orbit coupling, and thermal effects. *Physical Review B*, **2016**, 93,	3.3	33
222	Experimental and Theoretical High-Energy-Resolution X-ray Absorption Spectroscopy: Implications for the Investigation of the Entatic State. *Inorganic Chemistry*, **2016**, 55, 11694-11706	5.1	22
221	Vibration eigenmodes of the Au-(5□)/Si(111) surface studied by Raman spectroscopy and first-principles calculations. *Physical Review B*, **2016**, 94,	3.3	14
220	A Bifunctional Electrocatalyst for Oxygen Evolution and Oxygen Reduction Reactions in Water. *Angewandte Chemie*, **2016**, 128, 2396-2401	3.6	25
219	Temperature-Dependent Hole Mobility and Its Limit in Crystal-Phase P3HT Calculated from First Principles. *Journal of Physical Chemistry B*, **2016**, 120, 5572-80	3.4	9
218	Inhomogeneous and Homogeneous Line Broadening of Optical Spectra of PTCDA Molecules Adsorbed at Step Edges of Alkali Halide Surfaces. *Journal of Physical Chemistry C*, **2016**, 120, 11926-11937	3.8	8
217	Impurity-Mediated Early Condensation of a Charge Density Wave in an Atomic Wire Array. *ACS Nano*, **2016**, 10, 810-4	16.7	9

216	Manipulation resolves non-trivial structure of corrole monolayer on Ag(111). *Nanotechnology*, **2016**, 27, 025704	3.4	8
215	Solving the Scattering Problem for the P3HT On-Chain Charge Transport **2016**, 155-170		
214	Submonolayer Rare Earth Silicide Thin Films on the Si(111) Surface **2016**, 163-175		
213	LiTaO phonon dispersion and ferroelectric transition calculated from first principles. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 683-689	1.3	16
212	Density functional theory of the CuA -like Cu2 S2 diamond core in Cu 2II(NGuaS)2 Cl2. *Journal of Computational Chemistry*, **2016**, 37, 1005-18	3.5	12
211	A Bifunctional Electrocatalyst for Oxygen Evolution and Oxygen Reduction Reactions in Water. *Angewandte Chemie - International Edition*, **2016**, 55, 2350-5	16.4	102
210	Strain-induced quasi-one-dimensional rare-earth silicide structures on Si(111). *Physical Review B*, **2016**, 94,	3.3	8
209	Surface vibrational Raman modes of In:Si(111)(4□1) and (8□2) nanowires. *Physical Review B*, **2016**, 94,	3.3	13
208	Optical response of the Cu2 S2 diamond core in Cu2II(NGuaS)2 Cl2. *Journal of Computational Chemistry*, **2016**, 37, 2181-92	3.5	10
207	GaN m-plane: Atomic structure, surface bands, and optical response. *Physical Review B*, **2015**, 91,	3.3	39
206	Water adsorbate influence on the Cu(110) surface optical response. *Surface Science*, **2015**, 641, 231-236	1.8	8
205	Raman scattering efficiency in LiTaO3 and LiNbO3 crystals. *Physical Review B*, **2015**, 91,	3.3	59
204	Nanopatterning on H-Terminated Si(111) Explained as Dynamic Equilibrium of the Chemical Reaction with Methanol. *Journal of Physical Chemistry C*, **2015**, 119, 16947-16953	3.8	8
203	Liquid Crystal (8CB) Molecular Adsorption on Lithium Niobate Z-Cut Surfaces. *Journal of Physical Chemistry C*, **2015**, 119, 9342-9346	3.8	10
202	A panel of peralkylated sulfur□guanidine type bases: Novel pro-ligands for use in biomimetic coordination chemistry. *Inorganica Chimica Acta*, **2015**, 430, 225-238	2.7	5
201	Phonon dispersion and zero-point renormalization of LiNbO3 from density-functional perturbation theory. *Journal of Physics Condensed Matter*, **2015**, 27, 385402	1.8	23
200	Polaronic deformation at the Fe2+/3+ impurity site in Fe:LiNbO3 crystals. *Physical Review B*, **2015**, 91,	3.3	31
199	Interwire coupling for In(4□1)/Si(111) probed by surface transport. *Physical Review B*, **2015**, 92,	3.3	8

198	Mechanism for nuclear and electron spin excitation by radio frequency current. *Physical Review B*, **2015**, 92,	3.3	8
197	The Cu2O2 torture track for a real-life system: [Cu2(btmgp)2O2](2+) oxo and peroxo species in density functional calculations. *Journal of Computational Chemistry*, **2015**, 36, 1672-85	3.5	27
196	Barrier-free subsurface incorporation of 3d metal atoms into Bi(111) films. *Physical Review B*, **2015**, 91,	3.3	9
195	Influence of structural defects and oxidation onto hole conductivity in P3HT. *Journal of Physical Chemistry B*, **2015**, 119, 6481-91	3.4	10
194	Defect complexes in congruent LiNbO3 and their optical signatures. *Physical Review B*, **2015**, 91,	3.3	38
193	Structure formation in diindenoperylene thin films on copper(111). *Physical Chemistry Chemical Physics*, **2015**, 17, 8776-83	3.6	9
192	Surface Charge of Clean LiNbO3 Z-Cut Surfaces **2015**, 163-178		
191	Geometrical and optical benchmarking of copper guanidine-quinoline complexes: insights from TD-DFT and many-body perturbation theory. *Journal of Computational Chemistry*, **2014**, 35, 1-17	3.5	52
190	Modeling LiNbO3 Surfaces at Ambient Conditions. *Journal of Physical Chemistry C*, **2014**, 118, 10213-10220	3.8	12
189	Formation of Hydroxyl Groups at Calcium-Silicate-Hydrate (C-S-H): Coexistence of Ca□OH and Si□OH on Wollastonite(001). *Journal of Physical Chemistry C*, **2014**, 118, 8007-8013	3.8	23
188	The atomic structure of ternary amorphous TixSi1-xO2 hybrid oxides. *Journal of Physics Condensed Matter*, **2014**, 26, 253201	1.8	7
187	Adsorption of PTCDA on Terraces and at Steps Sites of the KCl(100) Surface. *Journal of Physical Chemistry C*, **2014**, 118, 29911-29918	3.8	20
186	Rashba splitting and relativistic energy shifts in In/Si(111) nanowires. *Physical Review B*, **2014**, 89,	3.3	18
185	Modeling intrinsic defects in LiNbO3 within the Slater-Janak transition state model. *Journal of Chemical Physics*, **2014**, 140, 234113	3.9	29
184	Oxygen adsorbates on the Si(111)4□1-In metallic atomic wire: Scanning tunneling microscopy and density-functional theory calculations. *Physical Review B*, **2014**, 90,	3.3	6
183	Unraveling the LiNbO3 X-cut surface by atomic force microscopy and density functional theory. *Physical Review B*, **2014**, 89,	3.3	7
182	Geometrical and optical benchmarking of copper(II) guanidine-quinoline complexes: insights from TD-DFT and many-body perturbation theory (part II). *Journal of Computational Chemistry*, **2014**, 35, 2146-61	3.5	26
181	Intrinsic LiNbO3 point defects from hybrid density functional calculations. *Physical Review B*, **2014**, 89,	3.3	33

180	Copper(110) surface in thermodynamic equilibrium with water vapor studied from first principles. *Surface Science*, **2013**, 612, 82-89	1.8	12
179	Monolayer Doping via Phosphonic Acid Grafting on Silicon: Microscopic Insight from Infrared Spectroscopy and Density Functional Theory Calculations. *Advanced Functional Materials*, **2013**, 23, 3471-3477	15.6	54
178	Vibrational Fingerprints of LiNbO3-LiTaO3 Mixed Crystals. *Ferroelectrics*, **2013**, 447, 63-68	0.6	7
177	LiNb1-xTaxO3 Electronic Structure and Optical Response from First-Principles Calculations. *Ferroelectrics*, **2013**, 447, 78-85	0.6	6
176	Transition energies and direct-indirect band gap crossing in zinc-blende AlxGa1□N. *Physical Review B*, **2013**, 87,	3.3	36
175	Optical response of stoichiometric and congruent lithium niobate from first-principles calculations. *Physical Review B*, **2013**, 87,	3.3	31
174	Structural variety of 5-fluoroarene-2-aminopyrimidine in comparison to 2-aminopyrimidine silver(I) coordination polymers: progress report and overview. *CrystEngComm*, **2013**, 15, 4225	3.3	12
173	Atomic structure of interface states in silicon heterojunction solar cells. *Physical Review Letters*, **2013**, 110, 136803	7.4	26
172	Bis-□xo and □2:2-peroxo dicopper complexes studied within (time-dependent) density-functional and many-body perturbation theory. *Journal of Computational Chemistry*, **2013**, 34, 1035-45	3.5	26
171	Frigge et al. reply. *Physical Review Letters*, **2013**, 111, 149602	7.4	8
170	Charge compensation by long-period reconstruction in strongly polar lithium niobate surfaces. *Physical Review B*, **2013**, 88,	3.3	21
169	Electronic and Optical Excitations of Aminopyrimidine Molecules from Many-Body Perturbation Theory **2013**, 17-28		
168	Lithium Niobate Dielectric Function and Second-Order Polarizability Tensor From Massively Parallel Ab Initio Calculations **2013**, 93-104		
167	Polarization Dependent Water Adsorption on the Lithium Niobate Z-Cut Surfaces **2013**, 155-166		
166	Polarization-dependent water adsorption on the LiNbO3(0001) surface. *Physical Review B*, **2012**, 86,	3.3	32
165	Linear and nonlinear optical response of LiNbO3 calculated from first principles. *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, **2012**, 59, 1929-33	3.2	9
164	Lithium niobate-tantalate mixed crystals electronic and optical properties calculated from first principles **2012**,		1
163	Ferroelectric phase transition in LiNbO3: Insights from molecular dynamics. *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, **2012**, 59, 1925-8	3.2	13

162	Substrate Induced Thermal Decomposition of Perfluoro-Pentacene Thin Films on the Coinage Metals. *Journal of Physical Chemistry C*, **2012**, 116, 24098-24106	3.8	21
161	pH-dependent structure and energetics of H2O/MgO(100). *Surface Science*, **2012**, 606, 902-907	1.8	22
160	Fingerprints of order and disorder in the electronic and optical properties of crystalline and amorphous TiO2. *Physical Review B*, **2012**, 86,	3.3	56
159	Activation of surface hydroxyl groups by modification of H-terminated Si(111) surfaces. *Journal of the American Chemical Society*, **2012**, 134, 8869-74	16.4	59
158	In-Si(111)(4 □1)/(8 □2) nanowires: Electron transport, entropy, and metal-insulator transition. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 343-359	1.3	21
157	Adsorption of OH and H at the LiNbO3(0001) surface. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2012**, 9, 1361-1365		14
156	The electronic structure and optical response of rutile, anatase and brookite TiO2. *Journal of Physics Condensed Matter*, **2012**, 24, 195503	1.8	357
155	2-Aminopyrimidine-silver(I) based organic semiconductors: Electronic structure and optical response. *Physical Review B*, **2012**, 85,	3.3	10
154	Atomic-resolution imaging of the polar (0001□) surface of LiNbO3 in aqueous solution by frequency modulation atomic force microscopy. *Physical Review B*, **2012**, 86,	3.3	31
153	Atomistic picture of charge density wave formation at surfaces. *Physical Review Letters*, **2012**, 109, 186101	7.4	58
152	Identification of the nitrogen split interstitial (N-N)(N) in GaN. *Physical Review Letters*, **2012**, 109, 206402	7.4	33
151	Polarization-dependent methanol adsorption on lithium niobate Z-cut surfaces. *Physical Review B*, **2012**, 86,	3.3	19
150	Copper Substrate Catalyzes Tetraazaperopyrene Polymerization **2012**, 47-56		
149	Entropy and Metal-Insulator Transition in Atomic-Scale Wires: The Case of In-Si(111)(4□1)/(8□2) **2012**, 131-139		
148	Vibrational properties of the LiNbO3 z-surfaces. *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, **2011**, 58, 1751-6	3.2	7
147	Group-VII point defects in ZnSe. *Physical Review B*, **2011**, 84,	3.3	10
146	Imaging of the Ferroelectric Domain Structures by Confocal Raman Spectroscopy. *Ferroelectrics*, **2011**, 420, 44-48	0.6	19
145	Photovoltaic applications of micro- and nano-crystalline silicon carbide. *Materials Research Society Symposia Proceedings*, **2011**, 1322, 51		1

144	Preserving charge and oxidation state of Au(III) ions in an agent-functionalized nanocrystal model system. *ACS Nano*, **2011**, 5, 6480-6	16.7	22
143	Asymmetric saddling of single porphyrin molecules on Au(111). *Physical Review B*, **2011**, 83,	3.3	23
142	Combined ab initio and classical potential simulation study on silicon carbide precipitation in silicon. *Physical Review B*, **2011**, 84,	3.3	16
141	Electrically detected electron-spin-echo envelope modulation: a highly sensitive technique for resolving complex interface structures. *Physical Review Letters*, **2011**, 106, 196101	7.4	25
140	Band offsets in cubic GaN/AlN superlattices. *Physical Review B*, **2011**, 83,	3.3	50
139	Barium titanate ground- and excited-state properties from first-principles calculations. *Physical Review B*, **2011**, 83,	3.3	65
138	Influence of Na adsorption on the quantum conductance and metal-insulator transition of the In-Si(111)(4□1)(8□2) nanowire array. *Physical Review B*, **2011**, 84,	3.3	16
137	Theoretical investigation of Er-O co-doping in hexagonal GaN. *Materials Research Society Symposia Proceedings*, **2011**, 1342, 73		1
136	Localised Phonon Modes at LiNbO3 (0001) Surfaces. *Ferroelectrics*, **2011**, 419, 1-8	0.6	8
135	Influence of Adatoms on the Quantum Conductance and Metal-Insulator Transition of Atomic-Scale Nanowires **2011**, 159-170		
134	Si(111)-In Nanowire Optical Response from Large-scale Ab Initio Calculations **2011**, 149-158		
133	Fine Structure of Triplet Centers in Room Temperature Irradiated 6H-SiC. *Materials Science Forum*, **2010**, 645-648, 403-406	0.4	3
132	Entropy explains metal-insulator transition of the Si(111)-In nanowire array. *Physical Review Letters*, **2010**, 105, 126102	7.4	73
131	First-principles study of water adsorption and a high-density interfacial ice structure on (1□1)-O/Rh(111). *Physical Review B*, **2010**, 82,	3.3	2
130	Chemical reactivity on surfaces: Modeling the imide synthesis from DATP and PTCDA on Au(111). *Physical Review B*, **2010**, 81,	3.3	11
129	Lithium niobate X-cut, Y-cut, and Z-cut surfaces from ab initio theory. *Physical Review B*, **2010**, 81,	3.3	103
128	Defects in carbon implanted silicon calculated by classical potentials and first-principles methods. *Physical Review B*, **2010**, 82,	3.3	6
127	Catalytic Action of a Cu(111) Surface on Tetraazaperopyrene Polymerization. *Journal of Physical Chemistry Letters*, **2010**, 1, 3266-3270	6.4	13

126	GaN/LiNbO3 (0 0 0 1) interface formation calculated from first-principles. *Applied Surface Science*, **2010**, 256, 5740-5743	6.7	7
125	Magnetic characterization of conductance electrons in GaN. *Physica Status Solidi (B): Basic Research*, **2010**, 247, 1728-1731	1.3	5
124	Ab initio investigation of the LiNbO3 (0001) surface. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2010**, 7, 145-148		12
123	Do we know the band gap of lithium niobate?. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2010**, 7, 362-365		77
122	GaN growth on LiNbO3 (0001) a first-principles simulation. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2010**, 7, 2272-2274		3
121	Understanding Electron Transport in Atomic Nanowires from Large-Scale Numerical Calculations **2010**, 233-242		
120	Understanding Long-range Indirect Interactions Between Surface Adsorbed Molecules **2010**, 75-84		
119	First-principles calculations of clean Au(110) surfaces and chemisorption of atomic oxygen. *Physical Review B*, **2009**, 79,	3.3	30
118	Adsorption structure of cyclopentene on InP(001)(2). *Physical Review B*, **2009**, 80,	3.3	7
117	Manganese-hydrogen complexes in Ga1MnxN. *Physical Review B*, **2009**, 80,	3.3	5
116	Structure of si(111)-in nanowires determined from the midinfrared optical response. *Physical Review Letters*, **2009**, 102, 226805	7.4	41
115	Glutamic acid adsorbed on Ag(110): direct and indirect molecular interactions. *Journal of Physics Condensed Matter*, **2009**, 21, 185001	1.8	9
114	Spin-Coupling in Heavily Nitrogen-Doped 4H-SiC. *Materials Science Forum*, **2009**, 615-617, 343-346	0.4	3
113	Optical anisotropy of the In/Si(111)(4)/(8) nanowire array. *Surface Science*, **2009**, 603, 247-250	1.8	9
112	Role of Dihydrogen Bonds for the Stabilization of Self-Assembled Molecular Nanostructures. *Journal of Physical Chemistry C*, **2009**, 113, 12653-12657	3.8	12
111	Chainlike Au Structures on Au(110)-(1) Surfaces Calculated from First Principles. *Journal of Physical Chemistry C*, **2009**, 113, 5690-5699	3.8	13
110	Water adsorption on the Al2O3(0001) surface. *Physical Review B*, **2009**, 80,	3.3	64
109	Rare-earth defect pairs in GaN: LDA+U calculations. *Physical Review B*, **2009**, 80,	3.3	64

108	Long-Range Chiral Recognition Due to Substrate Locking and Substrate-Adsorbate Charge Transfer **2009**, 641-648		
107	Understanding Molecular Recognition and Self-Assembly from Large-Scale Numerical Simulations **2009**, 129-137		
106	LiNbO3 ground- and excited-state properties from first-principles calculations. *Physical Review B*, **2008**, 77,	3.3	76
105	Influence of the Side Group Aromaticity on the Organic Molecule Adsorption on Cu(110). *Journal of Physical Chemistry C*, **2008**, 112, 11490-11494	3.8	7
104	Theoretical study of the localization of excess electrons at the surface of ice. *Journal of Physics Condensed Matter*, **2008**, 20, 225003	1.8	7
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