W Gero Schmidt

List of Publications by Citations

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	Semiempirical van der Waals correction to the density functional description of solids and molecular structures. *Physical Review B*, **2006**, 73,	3.3	641
286	The electronic structure and optical response of rutile, anatase and brookite TiO2. *Journal of Physics Condensed Matter*, **2012**, 24, 195503	1.8	357
285	Attracted by long-range electron correlation: adenine on graphite. *Physical Review Letters*, **2005**, 95, 186101	7.4	259
284	Efficient O(N2) method to solve the Bethe-Salpeter equation. *Physical Review B*, **2003**, 67,	3.3	121
283	Coulombic amino group-metal bonding: adsorption of adenine on Cu110. *Physical Review Letters*, **2005**, 94, 236102	7.4	120
282	Optical absorption of water: coulomb effects versus hydrogen bonding. *Physical Review Letters*, **2005**, 94, 037404	7.4	114
281	Bulk excitonic effects in surface optical spectra. *Physical Review Letters*, **2002**, 88, 016402	7.4	109
280	Lithium niobate X-cut, Y-cut, and Z-cut surfaces from ab initio theory. *Physical Review B*, **2010**, 81,	3.3	103
279	A Bifunctional Electrocatalyst for Oxygen Evolution and Oxygen Reduction Reactions in Water. *Angewandte Chemie - International Edition*, **2016**, 55, 2350-5	16.4	102
278	Reflectance Anisotropy of GaAs(100): Theory and Experiment. *Physical Review Letters*, **1998**, 81, 721-724	7.4	101
277	Geometry and electronic structure of GaAs(001)(2 x 4) reconstructions. *Physical Review B*, **1996**, 54, 16742-16748	3.3	88
276	Understanding reflectance anisotropy: Surface-state signatures and bulk-related features in the optical spectrum of InP(001)(2×4). *Physical Review B*, **2000**, 61, R16335-R16338	3.3	80
275	Ground- and excited-state properties of DNA base molecules from plane-wave calculations using ultrasoft pseudopotentials. *Journal of Computational Chemistry*, **2004**, 25, 112-22	3.5	79
274	Optically excited structural transition in atomic wires on surfaces at the quantum limit. *Nature*, **2017**, 544, 207-211	50.4	77
273	Do we know the band gap of lithium niobate?. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2010**, 7, 362-365		77
272	LiNbO3 ground- and excited-state properties from first-principles calculations. *Physical Review B*, **2008**, 77,	3.3	76
271	Surface phase diagram of (2×4) and (4×2) reconstructions of GaAs(001). *Physical Review B*, **2000**, 62, 8087-8091	3.3	74

270	Entropy explains metal-insulator transition of the Si(111)-In nanowire array. *Physical Review Letters*, **2010**, 105, 126102	7.4	73
269	Barium titanate ground- and excited-state properties from first-principles calculations. *Physical Review B*, **2011**, 83,	3.3	65
268	Water adsorption on the Al2O3(0001) surface. *Physical Review B*, **2009**, 80,	3.3	64
267	Rare-earth defect pairs in GaN: LDA+U calculations. *Physical Review B*, **2009**, 80,	3.3	64
266	Second-harmonic polarizability including electron-hole attraction from band-structure theory. *Physical Review B*, **2005**, 71,	3.3	63
265	Structure of the diamond (111) surface: Single-dangling-bond versus triple-dangling-bond face. *Physical Review B*, **1996**, 53, 13725-13733	3.3	62
264	Molecular electronic excitations calculated from a solid-state approach: Methodology and numerics. *Physical Review B*, **2005**, 72,	3.3	61
263	Organic molecule adsorption on solid surfaces: chemical bonding, mutual polarisation and dispersion interaction. *Applied Physics A: Materials Science and Processing*, **2006**, 85, 387-397	2.6	61
262	Strongly bonded water monomers on the ice Ih basal plane: Density-functional calculations. *Physical Review B*, **2006**, 74,	3.3	60
261	Terrace and step contributions to the optical anisotropy of Si(001) surfaces. *Physical Review B*, **2001**, 63,	3.3	60
260	Raman scattering efficiency in LiTaO3 and LiNbO3 crystals. *Physical Review B*, **2015**, 91,	3.3	59
259	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
258	Atomistic picture of charge density wave formation at surfaces. *Physical Review Letters*, **2012**, 109, 186101	7.4	58
257	Atomic structure of InP(001)-(2×4): A dimer reconstruction. *Physical Review B*, **1998**, 57, 14596-14599	3.3	58
256	Resolving the optical spectrum of water: coordination and electrostatic effects. *Physical Review Letters*, **2008**, 100, 207403	7.4	57
255	Quasiparticle bands and optical spectra of highly ionic crystals: AlN and NaCl. *Physical Review B*, **2005**, 72,	3.3	57
254	Geometrical and electronic structure of the reconstructed diamond (100) surface. *Physical Review B*, **1994**, 50, 17697-17700	3.3	57
253	Fingerprints of order and disorder in the electronic and optical properties of crystalline and amorphous TiO2. *Physical Review B*, **2012**, 86,	3.3	56

252	InP(001)-(2 x 1) surface: a hydrogen stabilized structure. *Physical Review Letters*, **2003**, 90, 126101	7.4	56
251	III-V(110) surface dynamics from an ab initio frozen-phonon approach. *Physical Review B*, **1995**, 52, 2001-2007	3.3	55
250	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
249	Hexagon versus trimer formation in in nanowires on Si(111): energetics and quantum conductance. *Physical Review Letters*, **2007**, 98, 026105	7.4	54
248	(2×4) GaP(001) surface: Atomic structure and optical anisotropy. *Physical Review B*, **1999**, 60, 2488-2494	3.3	54
247	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
246	Energetics of Si(001) surfaces exposed to electric fields and charge injection. *Physical Review Letters*, **2004**, 93, 036101	7.4	52
245	Ga-rich limit of surface reconstructions on GaAs(001): atomic structure of the (4 x 6) phase. *Physical Review Letters*, **2004**, 93, 266101	7.4	51
244	Band offsets in cubic GaN/AlN superlattices. *Physical Review B*, **2011**, 83,	3.3	50
243	Beyond the molecular movie: Dynamics of bands and bonds during a photoinduced phase transition. *Science*, **2018**, 362, 821-825	33.3	50
242	GaP(001) and InP(001): Reflectance anisotropy and surface geometry. *Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena*, **1999**, 17, 1691		47
241	Atomic Structure of the Sb-Stabilized GaAs(100)-(2 x 4) Surface. *Physical Review Letters*, **1996**, 77, 4402-4405	7.4	47
240	Chemisorption of antimony on GaAs(110). *Physical Review B*, **1994**, 49, 4731-4744	3.3	46
239	Structure of si(111)-in nanowires determined from the midinfrared optical response. *Physical Review Letters*, **2009**, 102, 226805	7.4	41
238	Long-range chiral recognition due to substrate locking and substrate-adsorbate charge transfer. *Physical Review Letters*, **2007**, 99, 196107	7.4	41
237	P-rich GaP(001)(2×1)/(2×1) surface: A hydrogen-adsorbate structure determined from first-principles calculations. *Physical Review B*, **2003**, 68,	3.3	40
236	GaN m-plane: Atomic structure, surface bands, and optical response. *Physical Review B*, **2015**, 91,	3.3	39
235	LiNbO surfaces from a microscopic perspective. *Journal of Physics Condensed Matter*, **2017**, 29, 413001	1.8	39

234	Defect complexes in congruent LiNbO3 and their optical signatures. *Physical Review B*, **2015**, 91,	3.3	38
233	X-ray diffraction analysis of the gallium-rich surface of GaAs(001). *Physical Review B*, **2001**, 64,	3.3	37
232	Structural fingerprints in the reflectance anisotropy spectra of InP(001)(2×4) surfaces. *Physical Review B*, **1999**, 59, 2234-2239	3.3	37
231	Transition energies and direct-indirect band gap crossing in zinc-blende AlxGa1−xN. *Physical Review B*, **2013**, 87,	3.3	36
230	Optical Properties of Ordered As Layers on InP(110) Surfaces. *Physical Review Letters*, **1996**, 77, 759-762	7.4	36
229	Optical anisotropy of the SiC((001))- (3x2) surface: evidence for the two-adlayer asymmetric-dimer model. *Physical Review Letters*, **2000**, 85, 4381-4	7.4	35
228	LiNbO3 electronic structure: Many-body interactions, spin-orbit coupling, and thermal effects. *Physical Review B*, **2016**, 93,	3.3	33
227	Intrinsic LiNbO3 point defects from hybrid density functional calculations. *Physical Review B*, **2014**, 89,	3.3	33
226	Identification of the nitrogen split interstitial (N-N)(N) in GaN. *Physical Review Letters*, **2012**, 109, 206402	7.4	33
225	Polarization-dependent water adsorption on the LiNbO3(0001) surface. *Physical Review B*, **2012**, 86,	3.3	32
224	Adatom-induced conductance modification of in nanowires: potential-well scattering and structural effects. *Physical Review Letters*, **2008**, 100, 106802	7.4	32
223	Polaronic deformation at the Fe2+/3+ impurity site in Fe:LiNbO3 crystals. *Physical Review B*, **2015**, 91,	3.3	31
222	Optical response of stoichiometric and congruent lithium niobate from first-principles calculations. *Physical Review B*, **2013**, 87,	3.3	31
221	Atomic-resolution imaging of the polar (0001̄) surface of LiNbO3 in aqueous solution by frequency modulation atomic force microscopy. *Physical Review B*, **2012**, 86,	3.3	31
220	First-principles calculations of clean Au(110) surfaces and chemisorption of atomic oxygen. *Physical Review B*, **2009**, 79,	3.3	30
219	Nanowire-induced optical anisotropy of the Si(111)-In surface. *Physical Review B*, **2003**, 68,	3.3	30
218	Chemisorption of pyrrole and polypyrrole on Si(001). *Physical Review B*, **2002**, 66,	3.3	30
217	Interplay of surface reconstruction and surface electric fields in the optical anisotropy of GaAs(001). *Physical Review B*, **2002**, 66,	3.3	30

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214	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
213	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
212	Atomic structure of interface states in silicon heterojunction solar cells. *Physical Review Letters*, **2013**, 110, 136803	7.4	26
211	Bis-□oxo 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
210	Organic modification of surface electronic properties: A first-principles study of uracil on Si(001). *Physical Review B*, **2004**, 69,	3.3	26
209	Understanding reflectance anisotropy: Surface-state signatures and bulk-related features. *Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena*, **2000**, 18, 2215		26
208	Rare-earth silicide thin films on the Si(111) surface. *Physical Review B*, **2016**, 93,	3.3	25
207	A Bifunctional Electrocatalyst for Oxygen Evolution and Oxygen Reduction Reactions in Water. *Angewandte Chemie*, **2016**, 128, 2396-2401	3.6	25
206	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
205	Understanding the optical anisotropy of oxidized Si(001) surfaces. *Physical Review B*, **2005**, 72,	3.3	25
204	Femtosecond transfer dynamics of photogenerated electrons at a surface resonance of reconstructed InP(100). *Physical Review Letters*, **2005**, 94, 067601	7.4	25
203	Gallium-rich reconstructions on GaAs(001). *Physica Status Solidi (B): Basic Research*, **2003**, 240, 91-98	1.3	25
202	Uracil Adsorbed on Si(001): Structure and Energetics. *Journal of Physical Chemistry B*, **2003**, 107, 5031-5035	3.4	25
201	Cycloaddition reaction versus dimer cleavage at the Si(001):C5H8 interface. *Physical Review B*, **2003**, 68,	3.3	25
200	Phenanthrenequinone adsorbed on Si(001): geometries, electronic properties, and optical response. *Journal of Physical Chemistry B*, **2005**, 109, 7928-33	3.4	24
199	SELF-ENERGY EFFECTS IN THE OPTICAL ANISOTROPY OF GaP(001). *Surface Review and Letters*, **1999**, 06, 1159-1165	1.1	24

198	Phonon dispersion and zero-point renormalization of LiNbO3 from density-functional perturbation theory. *Journal of Physics Condensed Matter*, **2015**, 27, 385402	1.8	23
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196	Asymmetric saddling of single porphyrin molecules on Au(111). *Physical Review B*, **2011**, 83,	3.3	23
195	Spatial modulation of molecular adsorption energies due to indirect interaction. *Physical Review B*, **2008**, 78,	3.3	23
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193	Steric effects and chirality in the adsorption of glycine and phenylglycine on Cu(110). *Nanotechnology*, **2007**, 18, 424030	3.4	23
192	The Bethe□Salpeter equation: a first-principles approach for calculating surface optical spectra. *Journal of Physics Condensed Matter*, **2004**, 16, S4313-S4322	1.8	23
191	Step-induced optical anisotropy of Si(111):H surfaces. *Physical Review B*, **2000**, 61, 7604-7608	3.3	23
190	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
189	pH-dependent structure and energetics of H2O/MgO(100). *Surface Science*, **2012**, 606, 902-907	1.8	22
188	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
187	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
186	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
185	Charge compensation by long-period reconstruction in strongly polar lithium niobate surfaces. *Physical Review B*, **2013**, 88,	3.3	21
184	Antimony-stabilized GaAs(001)(2□4) reconstructions. *Physical Review B*, **1997**, 55, 13051-13057	3.3	21
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182	Signatures of transient Wannier-Stark localization in bulk gallium arsenide. *Nature Communications*, **2018**, 9, 2890	17.4	20
181	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

180	Methyl Chloride Adsorption on Si(001)Electronic Structure. *Journal of Physical Chemistry B*, **2004**, 108, 7809-7813	3.4	20
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176	Imaging of the Ferroelectric Domain Structures by Confocal Raman Spectroscopy. *Ferroelectrics*, **2011**, 420, 44-48	0.6	19
175	Polarization-dependent methanol adsorption on lithium niobate Z-cut surfaces. *Physical Review B*, **2012**, 86,	3.3	19
174	Current density analysis of electron transport through molecular wires in open quantum systems. *Journal of Computational Chemistry*, **2017**, 38, 1685-1692	3.5	18
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172	Rashba splitting and relativistic energy shifts in In/Si(111) nanowires. *Physical Review B*, **2014**, 89,	3.3	18
171	Ga-rich GaAs(001) surface from ab initio calculations: Atomic structure of the (4) and (6) reconstructions. *Physical Review B*, **2006**, 73,	3.3	18
170	Calculation of reflectance anisotropy for semiconductor surface exploration. *Physica Status Solidi (B): Basic Research*, **2005**, 242, 2751-2764	1.3	18
169	Optical properties of Sb-terminated GaAs and InP (110) surfaces. *Physical Review B*, **1995**, 52, 12158-12167	3.3	17
168	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
167	Combined ab initio and classical potential simulation study on silicon carbide precipitation in silicon. *Physical Review B*, **2011**, 84,	3.3	16
166	Influence of Na adsorption on the quantum conductance and metal-insulator transition of the In-Si(111)(4)(3) nanowire array. *Physical Review B*, **2011**, 84,	3.3	16
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161	Vibrational properties of LiNb1−xTaxO3 mixed crystals. *Physical Review B*, **2016**, 93,	3.3	15
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159	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
158	Calculation of spin-spin zero-field splitting within periodic boundary conditions: Towards all-electron accuracy. *Physical Review B*, **2018**, 97,	3.3	14
157	Vibration eigenmodes of the Au-(5×2)/Si(111) surface studied by Raman spectroscopy and first-principles calculations. *Physical Review B*, **2016**, 94,	3.3	14
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155	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
154	Probing quasi-one-dimensional band structures by plasmon spectroscopy. *Physical Review B*, **2018**, 97,	3.3	13
153	Ferroelectric phase transition in LiNbO3: Insights from molecular dynamics. *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, **2012**, 59, 1925-8	3.2	13
152	Catalytic Action of a Cu(111) Surface on Tetraazaperopyrene Polymerization. *Journal of Physical Chemistry Letters*, **2010**, 1, 3266-3270	6.4	13
151	Chainlike Au□ Structures on Au(110)-(1 □) Surfaces Calculated from First Principles. *Journal of Physical Chemistry C*, **2009**, 113, 5690-5699	3.8	13
150	Ethanol adsorbed on ice: A first-principles study. *Physical Review B*, **2007**, 76,	3.3	13
149	Surface Ordering of P-rich InP(001): Hydrogen Stabilization vs Electron Correlation. *Surface Review and Letters*, **2003**, 10, 163-167	1.1	13
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147	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
146	Modeling LiNbO3 Surfaces at Ambient Conditions. *Journal of Physical Chemistry C*, **2014**, 118, 10213-10220	3.8	12
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144	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
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141	Energetics and Structure of Ordered Sb Overlayers and Sb Clusters on GaAs(110) Probed by ab initio Calculations. *Europhysics Letters*, **1994**, 25, 357-362	1.6	12
140	Si(775)-Au atomic chains: Geometry, optical properties, and spin order. *Physical Review Materials*, **2017**, 1,	3.2	12
139	Controlled growth of ordered monolayers of N-heterocyclic carbenes on silicon. *Nature Chemistry*, **2021**, 13, 828-835	17.6	12
138	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
137	Polytypism driven zero-field splitting of silicon vacancies in 6H-SiC. *Physical Review B*, **2018**, 98,	3.3	12
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134	Structural dynamics upon photoexcitation-induced charge transfer in a dicopper(i)-disulfide complex. *Physical Chemistry Chemical Physics*, **2018**, 20, 6274-6286	3.6	11
133	Chemical reactivity on surfaces: Modeling the imide synthesis from DATP and PTCDA on Au(111). *Physical Review B*, **2010**, 81,	3.3	11
132	Structure, energetics, and vibrational spectra of perylene adsorbed on Si(001): First-principles calculations compared with STM and HREELS. *Physical Review B*, **2006**, 74,	3.3	11
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129	Oxidation- and organic-molecule-induced changes of the Si surface optical anisotropy:ab initiopredictions. *Journal of Physics Condensed Matter*, **2004**, 16, S4323-S4334	1.8	11
128	Quasi-particle band structure of C(111)2 □1 and C(100)2 □1 surfaces. *Surface Science*, **1995**, 331-333, 1152-1156	1.8	11
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126	Spin pairing versus spin chains at Si(553)-Au surfaces. *Physical Review B*, **2018**, 98,	3.3	11
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123	Influence of structural defects and oxidation onto hole conductivity in P3HT. *Journal of Physical Chemistry B*, **2015**, 119, 6481-91	3.4	10
122	2-Aminopyrimidine-silver(I) based organic semiconductors: Electronic structure and optical response. *Physical Review B*, **2012**, 85,	3.3	10
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120	VUV-ellipsometry on GaN: Probing conduction band properties by core level excitations. *Physica Status Solidi (B): Basic Research*, **2005**, 242, 2601-2609	1.3	10
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118	Adatoms and vacancies on the diamond(111) surface. *Europhysics Letters*, **1996**, 35, 585-590	1.6	10
117	Optical response of the Cu2 S2 diamond core in Cu2II(NGuaS)2 Cl2. *Journal of Computational Chemistry*, **2016**, 37, 2181-92	3.5	10
116	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
115	Impurity-Mediated Early Condensation of a Charge Density Wave in an Atomic Wire Array. *ACS Nano*, **2016**, 10, 810-4	16.7	9
114	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
113	Barrier-free subsurface incorporation of 3d metal atoms into Bi(111) films. *Physical Review B*, **2015**, 91,	3.3	9
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111	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
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