Thomas Frauenheim

List of Publications by Year
in descending order

589	30,043	4641 85	7496 151
papers	citations	h-index	g-index

602	602	602	22883
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Monolayer PC3: A promising material for environmentally toxic nitrogen-containing multi gases. Journal of Hazardous Materials, 2022, 422, 126761.	6.5	25
2	Group three nitride clusters as promising components for nanoelectronics. Materials Today Chemistry, 2022, 23, 100751.	1.7	2
3	Dynamical evolution of the Schottky barrier as a determinant contribution to electronâ€“hole pair stabilization and photocatalysis of plasmon-induced hot carriers. Nanoscale, 2022, 14, 2816-2825.	2.8	11
4	Carrier doping-induced strong magnetoelastic coupling in 2D lattice. Nanoscale, 2022, 14, 3261-3268.	2.8	5
5	Universal co-existence of photovoltaics and ferroelectricity from a two-dimensional 3R bilayer BX (X) Tj ETQq1 1 0.784314 rgBT /Over	2.7	7
6	Fano Resonance and Incoherent Interlayer Excitons in Molecular van der Waals Heterostructures. Nano Letters, 2022, 22, 911-917.	4.5	4
7	Density functional tight binding approach utilized to study X-ray-induced transitions in solid materials. Scientific Reports, 2022, 12, 1551.	1.6	11
8	Plasmon-Enhanced Exciton Delocalization in Squaraine-Type Molecular Aggregates. ACS Nano, 2022, 16, 4693-4704.	7.3	6
9	Ultrafast Light-Induced Ferromagnetic State in Transition Metal Dichalcogenides Monolayers. Journal of Physical Chemistry Letters, 2022, 13, 2765-2771.	2.1	9
10	Transverse electronic transport through nucleobase-pairs of a DNA wire. Materials Today Chemistry, 2022, 24, 100834.	1.7	2
11	First-Principles Study of Honeycomb Borophene on the Mo₂C Substrate. Journal of Physical Chemistry C, 2022, 126, 7288-7293.	1.5	1
12	Tunable Surface Chemistry in Heterogeneous Bilayer Singleâ€Atom Catalysts for Electrocatalytic NO_x Reduction to Ammonia. Advanced Functional Materials, 2022, 32, .	7.8	30
13	Ultrahigh Electron Thermal Conductivity in Tâ€Graphene, Biphenylene, and Netâ€Graphene. Advanced Energy Materials, 2022, 12, .	10.2	26
14	Anisotropic Phononic and Electronic Thermal Transport in BeN₄. Journal of Physical Chemistry Letters, 2022, , 4501-4505.	2.1	5
15	Light-Controlled Ultrafast Magnetic State Transition in Antiferromagneticâ€“Ferromagnetic van der Waals Heterostructures. Journal of Physical Chemistry Letters, 2022, 13, 6223-6229.	2.1	5
16	Intermolecular conical intersections in molecular aggregates. Nature Nanotechnology, 2021, 16, 63-68.	15.6	22
17	Structural, electronic, and thermodynamic properties of TiO 2 /organic clusters: performance of DFTB method with different parameter sets. International Journal of Quantum Chemistry, 2021, 121, e26427.	1.0	7
18	Photoinduced charge-transfer in chromophore-labeled gold nanoclusters: quantum evidence of the critical role of ligands and vibronic couplings. Nanoscale, 2021, 13, 6786-6797.	2.8	8

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19	Possibilities and Limits of Decreasing the Gap of Anatase TiO₂ by Alloying with Nitrogen. Journal of Physical Chemistry C, 2021, 125, 3192-3197.	1.5	3
20	High-Throughput Screening of Synergistic Transition Metal Dual-Atom Catalysts for Efficient Nitrogen Fixation. Nano Letters, 2021, 21, 1871-1878.	4.5	223
21	Ni/Mo Bimetallicâ€Oxideâ€Derived Heterointerfaceâ€Rich Sulfide Nanosheets with Coâ€Doping for Efficient Alkaline Hydrogen Evolution by Boosting Volmer Reaction. Small, 2021, 17, e2006730.	5.2	95
22	Self-Consistent Potential Correction for Charged Periodic Systems. Physical Review Letters, 2021, 126, 076401.	2.9	44
23	Unravelling Photoinduced Interlayer Spin Transfer Dynamics in Two-Dimensional Nonmagnetic-Ferromagnetic van der Waals Heterostructures. Nano Letters, 2021, 21, 3237-3244.	4.5	29
24	Common Defects Accelerate Charge Separation and Reduce Recombination in CNT/Molecule Composites: Atomistic Quantum Dynamics. Journal of the American Chemical Society, 2021, 143, 6649-6656.	6.6	35
25	Possibility of Doping <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Cu</mml:mi><mml:mi>Ga</mml:mi><mml:mi>Se</mml:mi><mml:mn>2</mml:mn></mml:mrow><mml:mrow><mml:mi>n</mml:mi> -Type by Hydrogen. Physical Review Applied, 2021, 15, .	4.6	2
26	Identification of the Nitrogen Interstitial as Origin of the 3.1â€‰eV Photoluminescence Band in Hexagonal Boron Nitride. Physica Status Solidi (B): Basic Research, 2021, 258, 2100031.	0.7	3
27	Ultralow Thermal Conductivity in Two-Dimensional MoO₃. Nano Letters, 2021, 21, 4351-4356.	4.5	35
28	Electric Field Tunable Ultrafast Interlayer Charge Transfer in Graphene/WS₂ Heterostructure. Nano Letters, 2021, 21, 4403-4409.	4.5	15
29	New Pentaoctite Phase of Groupâ€V Nanostructures. Physica Status Solidi (B): Basic Research, 2021, 258, 2100112.	0.7	1
30	Revealing generation, migration, and dissociation of electron-hole pairs and current emergence in an organic photovoltaic cell. Science Advances, 2021, 7, .	4.7	15
31	Water Reactions on Reconstructed Rutile TiO₂: A Density Functional Theory/Density Functional Tight Binding Approach. Journal of Physical Chemistry C, 2021, 125, 13234-13246.	1.5	9
32	Using DFTB to Model Photocatalytic Anataseâ€“Rutile TiO2 Nanocrystalline Interfaces and Their Band Alignment. Journal of Chemical Theory and Computation, 2021, 17, 5239-5247.	2.3	3
33	Robust Giant Magnetoresistance in 2D Van der Waals Molecular Magnetic Tunnel Junctions. ACS Applied Materials & Interfaces, 2021, 13, 36098-36105.	4.0	8
34	Phononic Thermal Transport along Graphene Grain Boundaries: A Hidden Vulnerability. Advanced Science, 2021, 8, 2101624.	5.6	8
35	Construction of Nickelâ€Based Dual Heterointerfaces towards Accelerated Alkaline Hydrogen Evolution via Boosting Multiâ€Step Elementary Reaction. Advanced Functional Materials, 2021, 31, 2104827.	7.8	42
36	Activity and Mechanism Mapping of Photocatalytic NO2 Conversion on the Anatase TiO2(101) Surface. Journal of Physical Chemistry Letters, 2021, 12, 7708-7716.	2.1	7

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37	Tuning electronic and optical properties of bismuth monolayers by molecular adsorption. Surface Science, 2021, 710, 121849.	0.8	3
38	Artificial Intelligence Designer for Highly-Efficient Organic Photovoltaic Materials. Journal of Physical Chemistry Letters, 2021, 12, 8847-8854.	2.1	15
39	Stacking Engineering: A Boosting Strategy for 2D Photocatalysts. Journal of Physical Chemistry Letters, 2021, 12, 10190-10196.	2.1	25
40	Tuning Magnetic Anisotropy in Two-Dimensional Metalâ€“Semiconductor Janus van der Waals Heterostructures. Journal of Physical Chemistry Letters, 2021, 12, 11308-11315.	2.1	2
41	Electronic Properties of Defective MoS₂ Monolayers Subject to Mechanical Deformations: A Firstâ€Principles Approach. Physica Status Solidi (B): Basic Research, 2020, 257, 1900541.	0.7	8
42	Optically Driven Ultrafast Magnetic Order Transitions in Two-Dimensional Ferrimagnetic MXenes. Journal of Physical Chemistry Letters, 2020, 11, 6219-6226.	2.1	36
43	Ultrafast Real-Time Dynamics of CO Oxidation over an Oxide Photocatalyst. ACS Catalysis, 2020, 10, 13650-13658.	5.5	11
44	Electron paramagnetic resonance and theoretical study of gallium vacancy in Î² -Ga2O3. Applied Physics Letters, 2020, 117, .	1.5	33
45	Exploring charge density distribution and electronic properties of hybrid organic-germanium layers. Physical Chemistry Chemical Physics, 2020, 22, 22055-22065.	1.3	2
46	Electronic Properties and Charge Transfer of Topologically Protected States in Hybrid Bismuthene Layers. Journal of Physical Chemistry C, 2020, 124, 11708-11715.	1.5	6
47	GW electronic structure calculations of cobalt defects in ZnO. Solid State Communications, 2020, 316-317, 113950.	0.9	1
48	A Real-Time Time-Dependent Density Functional Tight-Binding Implementation for Semiclassical Excited State Electronâ€“Nuclear Dynamics and Pumpâ€“Probe Spectroscopy Simulations. Journal of Chemical Theory and Computation, 2020, 16, 4454-4469.	2.3	36
49	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	1.2	589
50	Inartificial Two-Dimensional Ge₄Se₉ Janus Structures with Appropriate Direct Band Gaps and Intrinsic Polarization Boosted Charge Separation for Photocatalytic Water Splitting. Journal of Physical Chemistry Letters, 2020, 11, 3095-3102.	2.1	26
51	An adaptive design approach for defects distribution modeling in materials from first-principle calculations. Journal of Molecular Modeling, 2020, 26, 187.	0.8	11
52	Koopmans-compliant screened exchange potential with correct asymptotic behavior for semiconductors. Physical Review B, 2020, 102, .	1.1	9
53	Intrinsic defects of GaSe. Journal of Physics Condensed Matter, 2020, 32, 285503.	0.7	4
54	Crystal structure and temperature-dependent properties of Na2H4Ga2GeO8Ââ€“ a novel gallogermanate. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2020, 75, 805-813.	0.3	0

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55	Densely-packed bundles of collapsed carbon nanotubes: Atomistic and mesoscopic distinct element method modeling. Carbon, 2019, 152, 198-205.	5.4	12
56	Optimized hybrid functionals for defect calculations in semiconductors. Journal of Applied Physics, 2019, 126, 130901.	1.1	27
57	Coherent Real-Space Charge Transport Across a Donorâ€“Acceptor Interface Mediated by Vibronic Couplings. Nano Letters, 2019, 19, 8630-8637.	4.5	14
58	Ultrafast Dynamics through a Conical Intersection in an Organic Photovoltaic Thin Film Probed by two-Dimensional Electronic Spectroscopy. , 2019, , .		0
59	Electronic and Optical Properties of Functionalized GaNâ€(101Â¯0) Surfaces using Hybridâ€Density Functionals. Physica Status Solidi (B): Basic Research, 2019, 256, 1800455.	0.7	2
60	Transition Metal and Rare Earth Element Doped Zinc Oxide Nanowires for Optoelectronics. Physica Status Solidi (B): Basic Research, 2019, 256, 1800604.	0.7	30
61	Dephasing in a Molecular Junction Viewed from a Time-Dependent and a Time-Independent Perspective. Journal of Physical Chemistry C, 2019, 123, 9590-9599.	1.5	5
62	SLABCC: Total energy correction code for charged periodic slab models. Computer Physics Communications, 2019, 240, 101-105.	3.0	9
63	Carbon in GaN: Calculations with an optimized hybrid functional. Physical Review B, 2019, 99, .	1.1	32
64	Plasmon-induced hot-carrier generation differences in gold and silver nanoclusters. Nanoscale, 2019, 11, 8604-8615.	2.8	51
65	Simulation of Impulsive Vibrational Spectroscopy. Journal of Physical Chemistry A, 2019, 123, 2065-2072.	1.1	10
66	Carrier multiplication in van der Waals layered transition metal dichalcogenides. Nature Communications, 2019, 10, 5488.	5.8	41
67	Defect calculations with hybrid functionals in layered compounds and in slab models. Physical Review B, 2019, 100, .	1.1	9
68	Collapsed carbon nanotubes: From nano to mesoscale via density functional theory-based tight-binding objective molecular modeling. Carbon, 2019, 143, 786-792.	5.4	12
69	Optoelectronic Properties of Zinc Oxide: A Firstâ€Principles Investigation Using the Tranâ€“Blaha Modified Beckeâ€“Johnson Potential. Physica Status Solidi (B): Basic Research, 2019, 256, 1800380.	0.7	6
70	Predicting Two-Dimensional C₃B/C₃N van der Waals pâ€“n Heterojunction with Strong Interlayer Electron Coupling and Enhanced Photocurrent. Journal of Physical Chemistry Letters, 2018, 9, 858-862.	2.1	74
71	Non-Markovian quantum processes: Complete framework and efficient characterization. Physical Review A, 2018, 97, .	1.0	202
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73	Origin of photoluminescence in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mo>â^'</mml:mo><mml:mi mathvariant="normal">G</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2018, 97, .	1.1	104
74	Exploring Surface Effects in Co Doped ZnO Nanowires With Hybridâ€Density Functional Theory. Physica Status Solidi (B): Basic Research, 2018, 255, 1800421.	0.7	1
75	Theoretical confirmation of the polaron model for the Mg acceptor in Î²-Ga2O3. Journal of Applied Physics, 2018, 124, .	1.1	34
76	Vibronic dephasing model for coherent-to-incoherent crossover in DNA. Physical Review B, 2018, 97, .	1.1	7
77	Fully Atomistic Real-Time Simulations of Transient Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2018, 9, 4355-4359.	2.1	21
78	Efficient Automatized Density-Functional Tight-Binding Parametrizations: Application to Group IV Elements. Journal of Chemical Theory and Computation, 2018, 14, 2947-2954.	2.3	18
79	Density functional based tight-binding parametrization of hafnium oxide: Simulations of amorphous structures. Physical Review B, 2018, 98, .	1.1	6
80	Core structure of dislocations in GaN revealed by transmission electron microscopy. , 2018, , 323-326.		0
81	Atomistic Analysis of Room Temperature Quantum Coherence in Two-Dimensional CdSe Nanostructures. Nano Letters, 2017, 17, 2389-2396.	4.5	29
82	Time-Dependent Extension of the Long-Range Corrected Density Functional Based Tight-Binding Method. Journal of Chemical Theory and Computation, 2017, 13, 1737-1747.	2.3	67
83	Choosing the correct hybrid for defect calculations: A case study on intrinsic carrier trapping in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î²</mml:mi><mml:mo>â^'</mml:mo><mml:mi mathvariant="normal">G</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physi	1.1	184
84	The spectral adjustment in nanoscale transport combined with the density functional based tight binding method. Computational Materials Science, 2017, 133, 14-21.	1.4	3
85	Charge transfer excitations from particle-particle random phase approximationâ€"Opportunities and challenges arising from two-electron deficient systems. Journal of Chemical Physics, 2017, 146, 124104.	1.2	10
86	Two-dimensional hydrogenated molybdenum and tungsten dinitrides MN₂H₂ (M = Mo, W) as novel quantum spin hall insulators with high stability. Nanoscale, 2017, 9, 1007-1013.	2.8	15
87	Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) Parameters for Ceria in 0D to 3D. Journal of Physical Chemistry C, 2017, 121, 4593-4607.	1.5	21
88	Optically and Electrically Controllable Adatom Spinâ€"orbital Dynamics in Transition Metal Dichalcogenides. Nano Letters, 2017, 17, 6721-6726.	4.5	4
89	Defect physics in intermediate-band materials: Insights from an optimized hybrid functional. Physical Review B, 2017, 96, .	1.1	13
90	Application of the Lanyâ€"Zunger polaron correction for calculating surface charge trapping. Journal of Physics Condensed Matter, 2017, 29, 394001.	0.7	11

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91	Properties of the Free-Standing Two-Dimensional Copper Monolayer. Journal of Nanomaterials, 2016, 2016, 1-6.	1.5	13
92	Coexistence of Three Ferroic Orders in the Multiferroic Compound [(CH₃)₄N][Mn(N₃)₃] with Perovskiteâ€Like Structure. Chemistry - A European Journal, 2016, 22, 7863-7870.	1.7	54
93	A Self Energy Model of Dephasing in Molecular Junctions. Journal of Physical Chemistry C, 2016, 120, 16383-16392.	1.5	12
94	Quantum mechanical modeling the emission pattern and polarization of nanoscale light emitting diodes. Nanoscale, 2016, 8, 13168-13173.	2.8	12
95	Novel Excitonic Solar Cells in Phosphoreneâ€“TiO₂ Heterostructures with Extraordinary Charge Separation Efficiency. Journal of Physical Chemistry Letters, 2016, 7, 1880-1887.	2.1	51
96	Two-dimensional rectangular tantalum carbide halides TaCX (X = Cl, Br, I): novel large-gap quantum spin Hall insulators. 2D Materials, 2016, 3, 035018.	2.0	21
97	A graphene-like Mg₃N₂monolayer: high stability, desirable direct band gap and promising carrier mobility. Physical Chemistry Chemical Physics, 2016, 18, 30379-30384.	1.3	29
98	Directional-dependent thickness and bending rigidity of phosphorene. Physical Review B, 2016, 94, .	1.1	16
99	Doped graphenes as anodes with large capacity for lithium-ion batteries. Journal of Materials Chemistry A, 2016, 4, 13407-13413.	5.2	57
100	Prediction of the quantum spin Hall effect in monolayers of transition-metal carbides MC (M = Ti, Zr,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.0	31
101	Many-body electronic structure calculations of Eu-doped ZnO. Physical Review B, 2016, 93, .	1.1	20
102	Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies. Journal of Physical Chemistry B, 2016, 120, 7297-7306.	1.2	52
103	Water splitting and the band edge positions of TiO2. Electrochimica Acta, 2016, 199, 27-34.	2.6	64
104	Nonadiabatic Molecular Dynamics for Thousand Atom Systems: A Tight-Binding Approach toward PYXAID. Journal of Chemical Theory and Computation, 2016, 12, 1436-1448.	2.3	93
105	Automatized Parameterization of the Densityâ€functional Tightâ€binding Method. II. Twoâ€center Integrals. Journal of the Chinese Chemical Society, 2016, 63, 57-68.	0.8	13
106	Light Absorption of Contacted Molecules: Insights and Impediments from Atomistic Simulations. Journal of Physical Chemistry C, 2016, 120, 3699-3704.	1.5	1
107	Driven Liouville von Neumann Equation in Lindblad Form. Journal of Physical Chemistry A, 2016, 120, 3278-3285.	1.1	33
108	New quantum spin Hall insulator in two-dimensional MoS₂with periodically distributed pores. Nanoscale, 2016, 8, 4915-4921.	2.8	20

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109	SiC₇siligraphene: a novel donor material with extraordinary sunlight absorption. Nanoscale, 2016, 8, 6994-6999.	2.8	70
110	Oxygen deficiency in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: Similarities and differences between the Ti self-interstitial and the O vacancy in bulk rutile and anatase. Physical Review B, 2015, 92, .	1.1	57
111	How the aggregation of oxygen vacancies in rutile-based<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math> causes memristive behavior. Physical Review B, 2015, 92, .	1.1	18
112	Atomic level simulation of permittivity of oxidized ultra-thin Si channels. , 2015, , .		0
113	SCCâ€ÐFTB parameters for simulating hybrid goldâ€thiolates compounds. Journal of Computational Chemistry, 2015, 36, 2075-2087.	1.5	82
114	Atomic level simulation of permittivity of oxidized ultra-thin si channels. , 2015, , .		0
115	Two-Dimensional Cu₂Si Monolayer with Planar Hexacoordinate Copper and Silicon Bonding. Journal of the American Chemical Society, 2015, 137, 2757-2762.	6.6	335
116	Robust Two-Dimensional Topological Insulators in Methyl-Functionalized Bismuth, Antimony, and Lead Bilayer Films. Nano Letters, 2015, 15, 1083-1089.	4.5	166
117	Nitrogen(II) Oxide Charge Transfer Complexes on TiO₂: A New Source for Visible-Light Activity. Journal of Physical Chemistry C, 2015, 119, 4488-4501.	1.5	33
118	Atomic Level Modeling of Extremely Thin Silicon-on-Insulator MOSFETs Including the Silicon Dioxide: Electronic Structure. IEEE Transactions on Electron Devices, 2015, 62, 696-704.	1.6	27
119	Proximity enhanced quantum spin Hall state in graphene. Carbon, 2015, 87, 418-423.	5.4	29
120	Extended Lagrangian Density Functional Tight-Binding Molecular Dynamics for Molecules and Solids. Journal of Chemical Theory and Computation, 2015, 11, 3357-3363.	2.3	26
121	The new dimension of silver. Physical Chemistry Chemical Physics, 2015, 17, 19695-19699.	1.3	52
122	Post-anti-van't Hoff-Le Bel motif in atomically thin germaniumâ€“copper alloy film. Physical Chemistry Chemical Physics, 2015, 17, 17545-17551.	1.3	81
123	Versatile Single-Layer Sodium Phosphidostannate(II): Strain-Tunable Electronic Structure, Excellent Mechanical Flexibility, and an Ideal Gap for Photovoltaics. Journal of Physical Chemistry Letters, 2015, 6, 2682-2687.	2.1	60
124	Accurate Hydrogen Bond Energies within the Density Functional Tight Binding Method. Journal of Physical Chemistry A, 2015, 119, 3535-3544.	1.1	20
125	Controllable magnetic correlation between two impurities by spin-orbit coupling in graphene. Scientific Reports, 2015, 5, 8943.	1.6	16
126	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. Journal of Physical Chemistry C, 2015, 119, 6918-6922.	1.5	210

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127	Narrow bandgap covalentâ€“organic frameworks with strong optical response in the visible and infrared. Journal of Materials Chemistry C, 2015, 3, 2244-2254.	2.7	18
128	Graphene-covered perovskites: an effective strategy to enhance light absorption and resist moisture degradation. RSC Advances, 2015, 5, 82346-82350.	1.7	43
129	Toward Rational Design of Catalysts Supported on a Topological Insulator Substrate. ACS Catalysis, 2015, 5, 7063-7067.	5.5	73
130	New Family of Quantum Spin Hall Insulators in Two-dimensional Transition-Metal Halide with Large Nontrivial Band Gaps. Nano Letters, 2015, 15, 7867-7872.	4.5	104
131	Ten new predicted covalent organic frameworks with strong optical response in the visible and near infrared. Journal of Chemical Physics, 2015, 142, 244706.	1.2	11
132	Controlling Electronic Structure and Transport Properties of Zigzag Graphene Nanoribbons by Edge Functionalization with Fluorine. Journal of Physical Chemistry C, 2015, 119, 21227-21233.	1.5	17
133	Permittivity of Oxidized Ultra-Thin Silicon Films From Atomistic Simulations. IEEE Electron Device Letters, 2015, 36, 1076-1078.	2.2	28
134	Resolving the Controversy about the Band Alignment between Rutile and Anatase: The Role of OH^{â€“}/H⁺ Adsorption. Journal of Physical Chemistry C, 2015, 119, 21952-21958.	1.5	43
135	Glitter in a 2D monolayer. Physical Chemistry Chemical Physics, 2015, 17, 26036-26042.	1.3	68
136	Revealing unusual chemical bonding in planar hyper-coordinate Ni₂Ge and quasi-planar Ni₂Si two-dimensional crystals. Physical Chemistry Chemical Physics, 2015, 17, 26043-26048.	1.3	95
137	Quantum spin Hall states in graphene interacting with WS2 or WSe2. Applied Physics Letters, 2014, 105, .	1.5	67
138	Phthalocyanine adsorption to graphene on Ir(111): Evidence for decoupling from vibrational spectroscopy. Journal of Chemical Physics, 2014, 141, 184308.	1.2	26
139	Publisher's Note: Formation of NV centers in diamond: A theoretical study based on calculated transitions and migration of nitrogen and vacancy related defects [Phys. Rev. B89, 075203 (2014)]. Physical Review B, 2014, 89, .	1.1	10
140	Reduction of the TiO_{2â€“x} melting temperature induced by oxygen deficiency with implications on experimental data accuracy and structural transition processes. Physica Status Solidi - Rapid Research Letters, 2014, 8, 549-553.	1.2	12
141	Charge-doping-induced phase transitions in hydrogenated and fluorinated graphene. Physical Review B, 2014, 90, .	1.1	4
142	Theoretical study of charge separation at the rutileâ€“anatase interface. Physica Status Solidi - Rapid Research Letters, 2014, 8, 566-570.	1.2	22
143	Preface: Focus on Functional Oxides. Physica Status Solidi - Rapid Research Letters, 2014, 8, 451-452.	1.2	5
144	Theoretical investigations of the electronic properties of functionalized zinc-oxide nanowires. Proceedings of SPIE, 2014, , .	0.8	0

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145	TiO2 Nanowires as a Wide Bandgap Dirac Material: a numerical study of impurity scattering and Anderson disorder. Materials Research Society Symposia Proceedings, 2014, 1659, 187-191.	0.1	0
146	Towards atomic level simulation of electron devices including the semiconductor-oxide interface. , 2014, , .		9
147	The dielectric response of low-k interlayer dielectric material characterized by electron energy loss spectroscopy. Microporous and Mesoporous Materials, 2014, 187, 23-28.	2.2	4
148	Strain engineering of selective chemical adsorption on monolayer MoS₂. Nanoscale, 2014, 6, 5156-5161.	2.8	177
149	Negative differential gain in quantum dot systems: Interplay of structural properties and many-body effects. Applied Physics Letters, 2014, 104, 242108.	1.5	8
150	Influence of porosity and methyl doping inside silica network: An electron diffraction and DFTB analysis. Microporous and Mesoporous Materials, 2014, 200, 145-150.	2.2	0
151	Robust 2D Topological Insulators in van der Waals Heterostructures. ACS Nano, 2014, 8, 10448-10454.	7.3	88
152	Formation of Helices in Graphene Nanoribbons under Torsion. Journal of Physical Chemistry Letters, 2014, 5, 4083-4087.	2.1	14
153	Polarons and oxygen vacancies at the surface of anatase TiO₂. Physica Status Solidi - Rapid Research Letters, 2014, 8, 583-586.	1.2	46
154	The role of water co-adsorption on the modification of ZnO nanowires using acetic acid. Physical Chemistry Chemical Physics, 2014, 16, 8509-8514.	1.3	8
155	Theoretical prediction of carbon dioxide reduction to methane at coordinatively unsaturated ferric site in the presence of Cu impurities. Physical Chemistry Chemical Physics, 2014, 16, 3515.	1.3	4
156	Opening a band gap without breaking lattice symmetry: a new route toward robust graphene-based nanoelectronics. Nanoscale, 2014, 6, 7474.	2.8	16
157	Proper Surface Termination for Luminescent Near-Surface NV Centers in Diamond. Nano Letters, 2014, 14, 4772-4777.	4.5	125
158	Structural Evolution of Cu/ZnO Active Sites: From Reactive Environment to Ultrahigh Vacuum. ChemCatChem, 2014, 6, 2322-2326.	1.8	5
159	Oxygen vacancy diffusion in bare ZnO nanowires. Nanoscale, 2014, 6, 11882-11886.	2.8	29
160	First principles investigations on the electronic structure of anchor groups on ZnO nanowires and surfaces. Journal of Applied Physics, 2014, 115, .	1.1	16
161	Phosphorene as a Superior Gas Sensor: Selective Adsorption and Distinct Iâ€“V Response. Journal of Physical Chemistry Letters, 2014, 5, 2675-2681.	2.1	877
162	Molecular dynamics simulations of the amino acid-ZnO (10-10) interface: A comparison between density functional theory and density functional tight binding results. Journal of Chemical Physics, 2014, 140, 234707.	1.2	11

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