Thomas Frauenheim

List of Publications by Year in Descending Order

574 papers	25,420 citations	78 h-index	139 g-index
602 ext. papers	27,733 ext. citations	4.6 avg, IF	7.06 L-index

#	Paper	IF	Citations
574	Dynamical evolution of the Schottky barrier as a determinant contribution to electron-hole pair stabilization and photocatalysis of plasmon-induced hot carriers.. *Nanoscale*, **2022**,	7.7	2
573	Universal co-existence of photovoltaics and ferroelectricity from a two-dimensional 3R bilayer BX (X = P, As, Sb). *Journal of Materials Chemistry C*, **2022**, 10, 1048-1061	7.1	0
572	Density functional tight binding approach utilized to study X-ray-induced transitions in solid materials.. *Scientific Reports*, **2022**, 12, 1551	4.9	1
571	Group three nitride clusters as promising components for nanoelectronics. *Materials Today Chemistry*, **2022**, 23, 100751	6.2	1
570	Monolayer PC: A promising material for environmentally toxic nitrogen-containing multi gases. *Journal of Hazardous Materials*, **2022**, 422, 126761	12.8	3
569	Ultrafast Light-Induced Ferromagnetic State in Transition Metal Dichalcogenides Monolayers.. *Journal of Physical Chemistry Letters*, **2022**, 2765-2771	6.4	1
568	Transverse electronic transport through nucleobase-pairs of a DNA wire. *Materials Today Chemistry*, **2022**, 24, 100834	6.2	1
567	Anisotropic Phononic and Electronic Thermal Transport in BeN.. *Journal of Physical Chemistry Letters*, **2022**, 4501-4505	6.4	1
566	Tuning Magnetic Anisotropy in Two-Dimensional Metal-Semiconductor Janus van der Waals Heterostructures. *Journal of Physical Chemistry Letters*, **2021**, 12, 11308-11315	6.4	0
565	Stacking Engineering: A Boosting Strategy for 2D Photocatalysts. *Journal of Physical Chemistry Letters*, **2021**, 12, 10190-10196	6.4	7
564	Unravelling Photoinduced Interlayer Spin Transfer Dynamics in Two-Dimensional Nonmagnetic-Ferromagnetic van der Waals Heterostructures. *Nano Letters*, **2021**, 21, 3237-3244	11.5	9
563	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	16.4	15
562	Identification of the Nitrogen Interstitial as Origin of the 3.1 eV Photoluminescence Band in Hexagonal Boron Nitride. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2100031	1.3	2
561	Ultralow Thermal Conductivity in Two-Dimensional MoO. *Nano Letters*, **2021**, 21, 4351-4356	11.5	16
560	Electric Field Tunable Ultrafast Interlayer Charge Transfer in Graphene/WS Heterostructure. *Nano Letters*, **2021**, 21, 4403-4409	11.5	4
559	New Pentaoctite Phase of Group-V Nanostructures. *Physica Status Solidi (B): Basic Research*, **2021**, 258, 2100112	1.3	0
558	Water Reactions on Reconstructed Rutile TiO2: A Density Functional Theory/Density Functional Tight Binding Approach. *Journal of Physical Chemistry C*, **2021**, 125, 13234-13246	3.8	4

557	Using DFTB to Model Photocatalytic Anatase-Rutile TiO Nanocrystalline Interfaces and Their Band Alignment. *Journal of Chemical Theory and Computation*, **2021**, 17, 5239-5247	6.4	0
556	Robust Giant Magnetoresistance in 2D Van der Waals Molecular Magnetic Tunnel Junctions. *ACS Applied Materials & Interfaces*, **2021**, 13, 36098-36105	9.5	3
555	Intermolecular conical intersections in molecular aggregates. *Nature Nanotechnology*, **2021**, 16, 63-68	28.7	7
554	Structural, electronic, and thermodynamic properties of TiO2/organic clusters: performance of DFTB method with different parameter sets. *International Journal of Quantum Chemistry*, **2021**, 121, e26427	2.1	1
553	Photoinduced charge-transfer in chromophore-labeled gold nanoclusters: quantum evidence of the critical role of ligands and vibronic couplings. *Nanoscale*, **2021**, 13, 6786-6797	7.7	1
552	Possibilities and Limits of Decreasing the Gap of Anatase TiO2 by Alloying with Nitrogen. *Journal of Physical Chemistry C*, **2021**, 125, 3192-3197	3.8	1
551	High-Throughput Screening of Synergistic Transition Metal Dual-Atom Catalysts for Efficient Nitrogen Fixation. *Nano Letters*, **2021**, 21, 1871-1878	11.5	66
550	Ni/Mo Bimetallic-Oxide-Derived Heterointerface-Rich Sulfide Nanosheets with Co-Doping for Efficient Alkaline Hydrogen Evolution by Boosting Volmer Reaction. *Small*, **2021**, 17, e2006730	11	32
549	Self-Consistent Potential Correction for Charged Periodic Systems. *Physical Review Letters*, **2021**, 126, 076401	7.4	14
548	Phononic Thermal Transport along Graphene Grain Boundaries: A Hidden Vulnerability. *Advanced Science*, **2021**, 8, e2101624	13.6	3
547	Activity and Mechanism Mapping of Photocatalytic NO Conversion on the Anatase TiO(101) Surface. *Journal of Physical Chemistry Letters*, **2021**, 12, 7708-7716	6.4	4
546	Tuning electronic and optical properties of bismuth monolayers by molecular adsorption. *Surface Science*, **2021**, 710, 121849	1.8	2
545	Artificial Intelligence Designer for Highly-Efficient Organic Photovoltaic Materials. *Journal of Physical Chemistry Letters*, **2021**, 12, 8847-8854	6.4	7
544	Electronic Properties and Charge Transfer of Topologically Protected States in Hybrid Bismuthene Layers. *Journal of Physical Chemistry C*, **2020**, 124, 11708-11715	3.8	4
543	GW electronic structure calculations of cobalt defects in ZnO. *Solid State Communications*, **2020**, 316-317, 113950	1.6	1
542	A Real-Time Time-Dependent Density Functional Tight-Binding Implementation for Semiclassical Excited State Electron-Nuclear Dynamics and Pump-Probe Spectroscopy Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 4454-4469	6.4	11
541	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *Journal of Chemical Physics*, **2020**, 152, 124101	3.9	210
540	Inartificial Two-Dimensional GeSe 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	6.4	10

539	An adaptive design approach for defects distribution modeling in materials from first-principle calculations. *Journal of Molecular Modeling*, **2020**, 26, 187	2	3
538	Koopmans-compliant screened exchange potential with correct asymptotic behavior for semiconductors. *Physical Review B*, **2020**, 102,	3.3	3
537	Intrinsic defects of GaSe. *Journal of Physics Condensed Matter*, **2020**, 32, 285503	1.8	1
536	Crystal structure and temperature-dependent properties of Na2H4Ga2GeO8 □a novel gallogermanate. *Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences*, **2020**, 75, 805-813	1	
535	Electronic Properties of Defective MoS2 Monolayers Subject to Mechanical Deformations: A First-Principles Approach. *Physica Status Solidi (B): Basic Research*, **2020**, 257, 1900541	1.3	5
534	Optically Driven Ultrafast Magnetic Order Transitions in Two-Dimensional Ferrimagnetic MXenes. *Journal of Physical Chemistry Letters*, **2020**, 11, 6219-6226	6.4	15
533	Ultrafast Real-Time Dynamics of CO Oxidation over an Oxide Photocatalyst. *ACS Catalysis*, **2020**, 10, 13650-13658	13.1	9
532	Electron paramagnetic resonance and theoretical study of gallium vacancy in □Ga2O3. *Applied Physics Letters*, **2020**, 117, 032101	3.4	19
531	Exploring charge density distribution and electronic properties of hybrid organic-germanium layers. *Physical Chemistry Chemical Physics*, **2020**, 22, 22055-22065	3.6	1
530	Electronic and Optical Properties of Functionalized GaN-(101□0) Surfaces using Hybrid-Density Functionals. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800455	1.3	2
529	Transition Metal and Rare Earth Element Doped Zinc Oxide Nanowires for Optoelectronics. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800604	1.3	21
528	Dephasing in a Molecular Junction Viewed from a Time-Dependent and a Time-Independent Perspective. *Journal of Physical Chemistry C*, **2019**, 123, 9590-9599	3.8	3
527	SLABCC: Total energy correction code for charged periodic slab models. *Computer Physics Communications*, **2019**, 240, 101-105	4.2	7
526	Carbon in GaN: Calculations with an optimized hybrid functional. *Physical Review B*, **2019**, 99,	3.3	24
525	Plasmon-induced hot-carrier generation differences in gold and silver nanoclusters. *Nanoscale*, **2019**, 11, 8604-8615	7.7	27
524	Densely-packed bundles of collapsed carbon nanotubes: Atomistic and mesoscopic distinct element method modeling. *Carbon*, **2019**, 152, 198-205	10.4	7
523	Optimized hybrid functionals for defect calculations in semiconductors. *Journal of Applied Physics*, **2019**, 126, 130901	2.5	12
522	Coherent Real-Space Charge Transport Across a Donor-Acceptor Interface Mediated by Vibronic Couplings. *Nano Letters*, **2019**, 19, 8630-8637	11.5	8

521	Simulation of Impulsive Vibrational Spectroscopy. *Journal of Physical Chemistry A*, **2019**, 123, 2065-2072	2.8	6
520	Carrier multiplication in van der Waals layered transition metal dichalcogenides. *Nature Communications*, **2019**, 10, 5488	17.4	18
519	Defect calculations with hybrid functionals in layered compounds and in slab models. *Physical Review B*, **2019**, 100,	3.3	8
518	Collapsed carbon nanotubes: From nano to mesoscale via density functional theory-based tight-binding objective molecular modeling. *Carbon*, **2019**, 143, 786-792	10.4	9
517	Optoelectronic Properties of Zinc Oxide: A First-Principles Investigation Using the TranBlaha Modified BeckeJohnson Potential. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800380	1.3	3
516	Predicting Two-Dimensional CB/CN van der Waals p-n Heterojunction with Strong Interlayer Electron Coupling and Enhanced Photocurrent. *Journal of Physical Chemistry Letters*, **2018**, 9, 858-862	6.4	55
515	Non-Markovian quantum processes: Complete framework and efficient characterization. *Physical Review A*, **2018**, 97,	2.6	114
514	Operational Markov Condition for Quantum Processes. *Physical Review Letters*, **2018**, 120, 040405	7.4	99
513	Origin of photoluminescence in Ga2O3. *Physical Review B*, **2018**, 97,	3.3	63
512	Fully Atomistic Real-Time Simulations of Transient Absorption Spectroscopy. *Journal of Physical Chemistry Letters*, **2018**, 9, 4355-4359	6.4	14
511	Efficient Automatized Density-Functional Tight-Binding Parametrizations: Application to Group IV Elements. *Journal of Chemical Theory and Computation*, **2018**, 14, 2947-2954	6.4	13
510	Density functional based tight-binding parametrization of hafnium oxide: Simulations of amorphous structures. *Physical Review B*, **2018**, 98,	3.3	4
509	Core structure of dislocations in GaN revealed by transmission electron microscopy **2018**, 323-326		
508	Exploring Surface Effects in Co Doped ZnO Nanowires With Hybrid-Density Functional Theory. *Physica Status Solidi (B): Basic Research*, **2018**, 255, 1800421	1.3	1
507	Theoretical confirmation of the polaron model for the Mg acceptor in Ga2O3. *Journal of Applied Physics*, **2018**, 124, 145702	2.5	24
506	Vibronic dephasing model for coherent-to-incoherent crossover in DNA. *Physical Review B*, **2018**, 97,	3.3	6
505	Atomistic Analysis of Room Temperature Quantum Coherence in Two-Dimensional CdSe Nanostructures. *Nano Letters*, **2017**, 17, 2389-2396	11.5	24
504	Time-Dependent Extension of the Long-Range Corrected Density Functional Based Tight-Binding Method. *Journal of Chemical Theory and Computation*, **2017**, 13, 1737-1747	6.4	46

503	Choosing the correct hybrid for defect calculations: A case study on intrinsic carrier trapping in Ga2O3. *Physical Review B*, **2017**, 95,	3.3	144
502	The spectral adjustment in nanoscale transport combined with the density functional based tight binding method. *Computational Materials Science*, **2017**, 133, 14-21	3.2	3
501	Charge transfer excitations from particle-particle random phase approximation-Opportunities and challenges arising from two-electron deficient systems. *Journal of Chemical Physics*, **2017**, 146, 124104	3.9	6
500	Two-dimensional hydrogenated molybdenum and tungsten dinitrides MNH (M = Mo, W) as novel quantum spin hall insulators with high stability. *Nanoscale*, **2017**, 9, 1007-1013	7.7	11
499	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	3.8	18
498	Optically and Electrically Controllable Adatom Spin-orbital Dynamics in Transition Metal Dichalcogenides. *Nano Letters*, **2017**, 17, 6721-6726	11.5	4
497	Defect physics in intermediate-band materials: Insights from an optimized hybrid functional. *Physical Review B*, **2017**, 96,	3.3	10
496	Application of the Lany-Zunger polaron correction for calculating surface charge trapping. *Journal of Physics Condensed Matter*, **2017**, 29, 394001	1.8	9
495	Prediction of the quantum spin Hall effect in monolayers of transition-metal carbides MC (M = Ti, Zr, Hf). *2D Materials*, **2016**, 3, 035022	5.9	21
494	Many-body electronic structure calculations of Eu-doped ZnO. *Physical Review B*, **2016**, 93,	3.3	20
493	Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies. *Journal of Physical Chemistry B*, **2016**, 120, 7297-306	3.4	42
492	Water splitting and the band edge positions of TiO2. *Electrochimica Acta*, **2016**, 199, 27-34	6.7	48
491	Nonadiabatic Molecular Dynamics for Thousand Atom Systems: A Tight-Binding Approach toward PYXAID. *Journal of Chemical Theory and Computation*, **2016**, 12, 1436-48	6.4	82
490	Automatized Parameterization of the Density-functional Tight-binding Method. II. Two-center Integrals. *Journal of the Chinese Chemical Society*, **2016**, 63, 57-68	1.5	11
489	Light Absorption of Contacted Molecules: Insights and Impediments from Atomistic Simulations. *Journal of Physical Chemistry C*, **2016**, 120, 3699-3704	3.8	1
488	Driven Liouville von Neumann Equation in Lindblad Form. *Journal of Physical Chemistry A*, **2016**, 120, 3278-85	2.8	25
487	New quantum spin Hall insulator in two-dimensional MoS2 with periodically distributed pores. *Nanoscale*, **2016**, 8, 4915-21	7.7	19
486	SiC7 siligraphene: a novel donor material with extraordinary sunlight absorption. *Nanoscale*, **2016**, 8, 6994-9	7.7	54

485	Properties of the Free-Standing Two-Dimensional Copper Monolayer. *Journal of Nanomaterials*, **2016**, 2016, 1-6	3.2	11
484	Coexistence of Three Ferroic Orders in the Multiferroic Compound [(CH3)4 N][Mn(N3)3] with Perovskite-Like Structure. *Chemistry - A European Journal*, **2016**, 22, 7863-70	4.8	46
483	A Self Energy Model of Dephasing in Molecular Junctions. *Journal of Physical Chemistry C*, **2016**, 120, 16383-16392	3.8	9
482	Quantum mechanical modeling the emission pattern and polarization of nanoscale light emitting diodes. *Nanoscale*, **2016**, 8, 13168-73	7.7	8
481	Novel Excitonic Solar Cells in Phosphorene-TiO2 Heterostructures with Extraordinary Charge Separation Efficiency. *Journal of Physical Chemistry Letters*, **2016**, 7, 1880-7	6.4	41
480	Two-dimensional rectangular tantalum carbide halides TaCX (X = Cl, Br, I): novel large-gap quantum spin Hall insulators. *2D Materials*, **2016**, 3, 035018	5.9	16
479	A graphene-like MgN monolayer: high stability, desirable direct band gap and promising carrier mobility. *Physical Chemistry Chemical Physics*, **2016**, 18, 30379-30384	3.6	24
478	Directional-dependent thickness and bending rigidity of phosphorene. *Physical Review B*, **2016**, 94,	3.3	14
477	Doped graphenes as anodes with large capacity for lithium-ion batteries. *Journal of Materials Chemistry A*, **2016**, 4, 13407-13413	13	47
476	Proximity enhanced quantum spin Hall state in graphene. *Carbon*, **2015**, 87, 418-423	10.4	26
475	Extended Lagrangian Density Functional Tight-Binding Molecular Dynamics for Molecules and Solids. *Journal of Chemical Theory and Computation*, **2015**, 11, 3357-63	6.4	19
474	The new dimension of silver. *Physical Chemistry Chemical Physics*, **2015**, 17, 19695-9	3.6	41
473	Post-anti-van't Hoff-Le Bel motif in atomically thin germanium-copper alloy film. *Physical Chemistry Chemical Physics*, **2015**, 17, 17545-51	3.6	65
472	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, 2682-7	6.4	48
471	Accurate hydrogen bond energies within the density functional tight binding method. *Journal of Physical Chemistry A*, **2015**, 119, 3535-44	2.8	17
470	Controllable magnetic correlation between two impurities by spin-orbit coupling in graphene. *Scientific Reports*, **2015**, 5, 8943	4.9	13
469	Structural and Electronic Properties of Layered Arsenic and Antimony Arsenide. *Journal of Physical Chemistry C*, **2015**, 119, 6918-6922	3.8	184
468	Narrow bandgap covalent organic frameworks with strong optical response in the visible and infrared. *Journal of Materials Chemistry C*, **2015**, 3, 2244-2254	7.1	15

467	Graphene-covered perovskites: an effective strategy to enhance light absorption and resist moisture degradation. *RSC Advances*, **2015**, 5, 82346-82350	3.7	40
466	Toward Rational Design of Catalysts Supported on a Topological Insulator Substrate. *ACS Catalysis*, **2015**, 5, 7063-7067	13.1	43
465	New Family of Quantum Spin Hall Insulators in Two-dimensional Transition-Metal Halide with Large Nontrivial Band Gaps. *Nano Letters*, **2015**, 15, 7867-72	11.5	87
464	Ten new predicted covalent organic frameworks with strong optical response in the visible and near infrared. *Journal of Chemical Physics*, **2015**, 142, 244706	3.9	10
463	Controlling Electronic Structure and Transport Properties of Zigzag Graphene Nanoribbons by Edge Functionalization with Fluorine. *Journal of Physical Chemistry C*, **2015**, 119, 21227-21233	3.8	15
462	Permittivity of Oxidized Ultra-Thin Silicon Films From Atomistic Simulations. *IEEE Electron Device Letters*, **2015**, 36, 1076-1078	4.4	11
461	Resolving the Controversy about the Band Alignment between Rutile and Anatase: The Role of OH⁄H+ Adsorption. *Journal of Physical Chemistry C*, **2015**, 119, 21952-21958	3.8	42
460	Glitter in a 2D monolayer. *Physical Chemistry Chemical Physics*, **2015**, 17, 26036-42	3.6	54
459	Revealing unusual chemical bonding in planar hyper-coordinate Ni2Ge and quasi-planar Ni2Si two-dimensional crystals. *Physical Chemistry Chemical Physics*, **2015**, 17, 26043-8	3.6	73
458	Oxygen deficiency in TiO2: Similarities and differences between the Ti self-interstitial and the O vacancy in bulk rutile and anatase. *Physical Review B*, **2015**, 92,	3.3	49
457	How the aggregation of oxygen vacancies in rutile-based TiO2□ phases causes memristive behavior. *Physical Review B*, **2015**, 92,	3.3	11
456	SCC-DFTB parameters for simulating hybrid gold-thiolates compounds. *Journal of Computational Chemistry*, **2015**, 36, 2075-87	3.5	58
455	Two-dimensional Cu2Si monolayer with planar hexacoordinate copper and silicon bonding. *Journal of the American Chemical Society*, **2015**, 137, 2757-62	16.4	237
454	Robust two-dimensional topological insulators in methyl-functionalized bismuth, antimony, and lead bilayer films. *Nano Letters*, **2015**, 15, 1083-9	11.5	145
453	Nitrogen(II) Oxide Charge Transfer Complexes on TiO2: A New Source for Visible-Light Activity. *Journal of Physical Chemistry C*, **2015**, 119, 4488-4501	3.8	29
452	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	2.9	17
451	Strain engineering of selective chemical adsorption on monolayer MoS2. *Nanoscale*, **2014**, 6, 5156-61	7.7	148
450	Negative differential gain in quantum dot systems: Interplay of structural properties and many-body effects. *Applied Physics Letters*, **2014**, 104, 242108	3.4	6

449	Influence of porosity and methyl doping inside silica network: An electron diffraction and DFTB analysis. *Microporous and Mesoporous Materials*, **2014**, 200, 145-150	5.3	
448	Robust 2D topological insulators in van der Waals heterostructures. *ACS Nano*, **2014**, 8, 10448-54	16.7	74
447	Formation of Helices in Graphene Nanoribbons under Torsion. *Journal of Physical Chemistry Letters*, **2014**, 5, 4083-7	6.4	13
446	Polarons and oxygen vacancies at the surface of anatase TiO2. *Physica Status Solidi - Rapid Research Letters*, **2014**, 8, 583-586	2.5	36
445	The role of water co-adsorption on the modification of ZnO nanowires using acetic acid. *Physical Chemistry Chemical Physics*, **2014**, 16, 8509-14	3.6	8
444	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, 3515-9	3.6	4
443	Opening a band gap without breaking lattice symmetry: a new route toward robust graphene-based nanoelectronics. *Nanoscale*, **2014**, 6, 7474-9	7.7	11
442	Proper surface termination for luminescent near-surface NV centers in diamond. *Nano Letters*, **2014** , 14, 4772-7	11.5	92
441	Structural Evolution of Cu/ZnO Active Sites: From Reactive Environment to Ultrahigh Vacuum. *ChemCatChem*, **2014**, 6, 2322-2326	5.2	5
440	Oxygen vacancy diffusion in bare ZnO nanowires. *Nanoscale*, **2014**, 6, 11882-6	7.7	24
439	First principles investigations on the electronic structure of anchor groups on ZnO nanowires and surfaces. *Journal of Applied Physics*, **2014**, 115, 203720	2.5	16
438	Phosphorene as a Superior Gas Sensor: Selective Adsorption and Distinct I-V Response. *Journal of Physical Chemistry Letters*, **2014**, 5, 2675-81	6.4	723
437	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	3.9	9
436	Formation of NV centers in diamond: A theoretical study based on calculated transitions and migration of nitrogen and vacancy related defects. *Physical Review B*, **2014**, 89,	3.3	113
435	Stabilization mechanism of ZnO nanoparticles by Fe doping. *Physical Review Letters*, **2014**, 112, 106102	7.4	20
434	Graphene nucleation on a surface-molten copper catalyst: quantum chemical molecular dynamics simulations. *Chemical Science*, **2014**, 5, 3493-3500	9.4	36
433	Polar EuO(111) on Ir(111): A two-dimensional oxide. *Physical Review B*, **2014**, 89,	3.3	4
432	Intense intrashell luminescence of Eu-doped single ZnO nanowires at room temperature by implantation created Eu-Oi complexes. *Nano Letters*, **2014**, 14, 4523-8	11.5	60

431	CO2 reduction at low overpotential on Cu electrodes in the presence of impurities at the subsurface. *Journal of Materials Chemistry A*, **2014**, 2, 4885-4889	13	32
430	The atomic structure of ternary amorphous TixSi1-xO2 hybrid oxides. *Journal of Physics Condensed Matter*, **2014**, 26, 253201	1.8	7
429	Quantum spin Hall states in graphene interacting with WS2 or WSe2. *Applied Physics Letters*, **2014**, 105, 233112	3.4	57
428	Phthalocyanine adsorption to graphene on Ir(111): evidence for decoupling from vibrational spectroscopy. *Journal of Chemical Physics*, **2014**, 141, 184308	3.9	25
427	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. B 89, 075203 (2014)]. *Physical Review B*, **2014**, 89,	3.3	8
426	Reduction of the TiO2 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	2.5	12
425	Charge-doping-induced phase transitions in hydrogenated and fluorinated graphene. *Physical Review B*, **2014**, 90,	3.3	2
424	Theoretical study of charge separation at the rutile anatase interface. *Physica Status Solidi - Rapid Research Letters*, **2014**, 8, 566-570	2.5	20
423	Preface: Focus on Functional Oxides. *Physica Status Solidi - Rapid Research Letters*, **2014**, 8, 451-452	2.5	1
422	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		
421	Towards atomic level simulation of electron devices including the semiconductor-oxide interface **2014**,		4
420	The dielectric response of low-k interlayer dielectric material characterized by electron energy loss spectroscopy. *Microporous and Mesoporous Materials*, **2014**, 187, 23-28	5.3	2
419	Parameterization of Halogens for the Density-Functional Tight-Binding Description of Halide Hydration. *Journal of Chemical Theory and Computation*, **2013**, 9, 3321-32	6.4	11
418	Fe-doped ZnO nanoparticles: the oxidation number and local charge on iron, studied by 57Fe MBauer spectroscopy and DFT calculations. *Chemistry - A European Journal*, **2013**, 19, 3287-91	4.8	24
417	Signatures in vibrational and UV-visible absorption spectra for identifying cyclic hydrocarbons by graphene fragments. *Nanoscale*, **2013**, 5, 12178-84	7.7	15
416	Graphene-based topological insulator with an intrinsic bulk band gap above room temperature. *Nano Letters*, **2013**, 13, 6251-5	11.5	102
415	Extensions of the Time-Dependent Density Functional Based Tight-Binding Approach. *Journal of Chemical Theory and Computation*, **2013**, 9, 4901-14	6.4	51
414	Computational approach for structure design and prediction of optical properties in amorphous TiO2thin-film coatings. *Journal Physics D: Applied Physics*, **2013**, 46, 325302	3	27

413	Controllable magnetic doping of the surface state of a topological insulator. *Physical Review Letters*, **2013**, 110, 126804	7.4	90
412	How small nanodiamonds can be? MD study of the stability against graphitization. *Diamond and Related Materials*, **2013**, 33, 78-84	3.5	8
411	Temperature-Mediated Magnetism in Fe-Doped ZnO Semiconductors. *Journal of Physical Chemistry C*, **2013**, 117, 5338-5342	3.8	16
410	Atomistic Modeling of Charge Transport across a Carbon Nanotube–Polyethylene Junction. *Journal of Physical Chemistry C*, **2013**, 117, 8020-8027	3.8	12
409	Gas doping on the topological insulator Bi2Se3 surface. *Physical Review Letters*, **2013**, 110, 016403	7.4	26
408	Intrinsic Charge Separation and Tunable Electronic Band Gap of Armchair Graphene Nanoribbons Encapsulated in a Double-Walled Carbon Nanotube. *Journal of Physical Chemistry Letters*, **2013**, 4, 1328-33	6.4	12
407	Emergent properties and trends of a new class of carbon nanocomposites: graphene nanoribbons encapsulated in a carbon nanotube. *Nanoscale*, **2013**, 5, 3306-14	7.7	10
406	Parametrization of the SCC-DFTB Method for Halogens. *Journal of Chemical Theory and Computation*, **2013**, 9, 2939-49	6.4	45
405	Theoretical Insights into CO2 Activation and Reduction on the Ag(111) Monolayer Supported on a ZnO(0001) Substrate. *Journal of Physical Chemistry C*, **2013**, 117, 1804-1808	3.8	45
404	Nanoscale Multilayer Transition-Metal Dichalcogenide Heterostructures: Band Gap Modulation by Interfacial Strain and Spontaneous Polarization. *Journal of Physical Chemistry Letters*, **2013**, 4, 1730-6	6.4	126
403	An SCC-DFTB Repulsive Potential for Various ZnO Polymorphs and the ZnO-Water System. *Journal of Physical Chemistry C*, **2013**, 117, 17004-17015	3.8	35
402	Possibility of a field effect transistor based on Dirac particles in semiconducting anatase-TiO2 nanowires. *Nano Letters*, **2013**, 13, 1073-9	11.5	10
401	Magnetic impurity affected by spin-orbit coupling: Behavior near a topological phase transition. *Physical Review B*, **2013**, 88,	3.3	7
400	Molecular dynamics simulations of the tribological behaviour of a water-lubricated amorphous carbon–fluorine PECVD coating. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 055027	2	3
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