

Jin-Long Yang

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533
ext. papers

33,296
ext. citations

7.9
avg, IF

7.63
L-index

#	Paper	IF	Citations
503	Partially oxidized atomic cobalt layers for carbon dioxide electroreduction to liquid fuel. <i>Nature</i> , 2016 , 529, 68-71	50.4	1231
502	Metallic few-layered VS ₂ ultrathin nanosheets: high two-dimensional conductivity for in-plane supercapacitors. <i>Journal of the American Chemical Society</i> , 2011 , 133, 17832-8	16.4	886
501	Regulation of Coordination Number over Single Co Sites: Triggering the Efficient Electroreduction of CO. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 1944-1948	16.4	607
500	Half-metallicity in edge-modified zigzag graphene nanoribbons. <i>Journal of the American Chemical Society</i> , 2008 , 130, 4224-5	16.4	587
499	Two-dimensional boron monolayer sheets. <i>ACS Nano</i> , 2012 , 6, 7443-53	16.7	548
498	Controlling the Kondo effect of an adsorbed magnetic ion through its chemical bonding. <i>Science</i> , 2005 , 309, 1542-4	33.3	543
497	Identification of single-atom active sites in carbon-based cobalt catalysts during electrocatalytic hydrogen evolution. <i>Nature Catalysis</i> , 2019 , 2, 134-141	36.5	409
496	Giant moisture responsiveness of VS ₂ ultrathin nanosheets for novel touchless positioning interface. <i>Advanced Materials</i> , 2012 , 24, 1969-74	24	324
495	Bottom-up precise synthesis of stable platinum dimers on graphene. <i>Nature Communications</i> , 2017 , 8, 1070	17.4	306
494	Low-temperature growth of graphene by chemical vapor deposition using solid and liquid carbon sources. <i>ACS Nano</i> , 2011 , 5, 3385-90	16.7	304
493	Enhanced photocatalytic mechanism for the hybrid g-C ₃ N ₄ /MoS ₂ nanocomposite. <i>Journal of Materials Chemistry A</i> , 2014 , 2, 7960-7966	13	289
492	How graphene is cut upon oxidation?. <i>Journal of the American Chemical Society</i> , 2009 , 131, 6320-1	16.4	289
491	Will zigzag graphene nanoribbon turn to half metal under electric field?. <i>Applied Physics Letters</i> , 2007 , 91, 243116	3.4	285
490	First-Principles Thermodynamics of Graphene Growth on Cu Surfaces. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 17782-17787	3.8	276
489	Half-metallicity in MnPSe ₂ exfoliated nanosheet with carrier doping. <i>Journal of the American Chemical Society</i> , 2014 , 136, 11065-9	16.4	264
488	CrXTe ₃ (X = Si, Ge) nanosheets: two dimensional intrinsic ferromagnetic semiconductors. <i>Journal of Materials Chemistry C</i> , 2014 , 2, 7071	7.1	262
487	Atomically dispersed iron hydroxide anchored on Pt for preferential oxidation of CO in H ₂ . <i>Nature</i> , 2019 , 565, 631-635	50.4	260

486	Understanding of Strain Effects in the Electrochemical Reduction of CO : Using Pd Nanostructures as an Ideal Platform. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 3594-3598	16.4	229
485	Hydrogen-incorporated TiS ₂ ultrathin nanosheets with ultrahigh conductivity for stamp-transferrable electrodes. <i>Journal of the American Chemical Society</i> , 2013 , 135, 5144-51	16.4	228
484	Wet electrons at the H ₂ O/TiO ₂ (110) surface. <i>Science</i> , 2005 , 308, 1154-8	33.3	214
483	Visualizing coherent intermolecular dipole-dipole coupling in real space. <i>Nature</i> , 2016 , 531, 623-7	50.4	213
482	Conjugated Microporous Polymer Nanosheets for Overall Water Splitting Using Visible Light. <i>Advanced Materials</i> , 2017 , 29, 1702428	24	211
481	Achieving Remarkable Activity and Durability toward Oxygen Reduction Reaction Based on Ultrathin Rh-Doped Pt Nanowires. <i>Journal of the American Chemical Society</i> , 2017 , 139, 8152-8159	16.4	210
480	Structural isomerism in gold nanoparticles revealed by X-ray crystallography. [Corrected]. <i>Nature Communications</i> , 2015 , 6, 8667	17.4	208
479	Obtaining two-dimensional electron gas in free space without resorting to electron doping: an electronegative based design. <i>Journal of the American Chemical Society</i> , 2014 , 136, 13313-8	16.4	204
478	Graphene nanoribbon as a negative differential resistance device. <i>Applied Physics Letters</i> , 2009 , 94, 17313-4	11.0	204
477	Distinguishing adjacent molecules on a surface using plasmon-enhanced Raman scattering. <i>Nature Nanotechnology</i> , 2015 , 10, 865-9	28.7	202
476	Electronic structures of SiC nanoribbons. <i>Journal of Chemical Physics</i> , 2008 , 129, 174114	3.9	199
475	Oxygen molecule dissociation on carbon nanostructures with different types of nitrogen doping. <i>Nanoscale</i> , 2012 , 4, 1184-9	7.7	195
474	Dynamic oxygen adsorption on single-atomic Ruthenium catalyst with high performance for acidic oxygen evolution reaction. <i>Nature Communications</i> , 2019 , 10, 4849	17.4	194
473	First-principles design of spintronics materials. <i>National Science Review</i> , 2016 , 3, 365-381	10.8	191
472	Ultrafast interfacial proton-coupled electron transfer. <i>Science</i> , 2006 , 311, 1436-40	33.3	185
471	One-dimensional transition metal-benzene sandwich polymers: possible ideal conductors for spin transport. <i>Journal of the American Chemical Society</i> , 2006 , 128, 2310-4	16.4	185
470	Defects in Phosphorene. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 20474-20480	3.8	183
469	Atomic-Level Insight into Optimizing the Hydrogen Evolution Pathway over a Co -N Single-Site Photocatalyst. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 12191-12196	16.4	183

468	The electronic structure of oxygen atom vacancy and hydroxyl impurity defects on titanium dioxide (110) surface. <i>Journal of Chemical Physics</i> , 2009 , 130, 124502	3.9	183
467	A theoretical study of single-atom catalysis of CO oxidation using Au embedded 2D h-BN monolayer: a CO-promoted O ₂ activation. <i>Scientific Reports</i> , 2014 , 4, 5441	4.9	177
466	Highly Efficient Photocatalytic Water Splitting over Edge-Modified Phosphorene Nanoribbons. <i>Journal of the American Chemical Society</i> , 2017 , 139, 15429-15436	16.4	176
465	Regulation of Coordination Number over Single Co Sites: Triggering the Efficient Electroreduction of CO ₂ . <i>Angewandte Chemie</i> , 2018 , 130, 1962-1966	3.6	176
464	Silicene as a highly sensitive molecule sensor for NH ₃ , NO and NO ₂ . <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 6957-62	3.6	173
463	A first-principles study of gas adsorption on germanene. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 22495-8	3.6	172
462	Single Mo1(Cr1) Atom on Nitrogen-Doped Graphene Enables Highly Selective Electroreduction of Nitrogen into Ammonia. <i>ACS Catalysis</i> , 2019 , 9, 3419-3425	13.1	170
461	Mono-Mercury Doping of Au ₂₅ and the HOMO/LUMO Energies Evaluation Employing Differential Pulse Voltammetry. <i>Journal of the American Chemical Society</i> , 2015 , 137, 9511-4	16.4	168
460	Intrinsic Electric Fields in Two-dimensional Materials Boost the Solar-to-Hydrogen Efficiency for Photocatalytic Water Splitting. <i>Nano Letters</i> , 2018 , 18, 6312-6317	11.5	168
459	Proposed photosynthesis method for producing hydrogen from dissociated water molecules using incident near-infrared light. <i>Physical Review Letters</i> , 2014 , 112, 018301	7.4	163
458	Bipolar magnetic semiconductors: a new class of spintronics materials. <i>Nanoscale</i> , 2012 , 4, 5680-5	7.7	162
457	Role of point defects on the reactivity of reconstructed anatase titanium dioxide (001) surface. <i>Nature Communications</i> , 2013 , 4, 2214	17.4	162
456	Mono-cadmium vs Mono-mercury Doping of Au ₂₅ Nanoclusters. <i>Journal of the American Chemical Society</i> , 2015 , 137, 15350-3	16.4	159
455	Strain effect on electronic structures of graphene nanoribbons: A first-principles study. <i>Journal of Chemical Physics</i> , 2008 , 129, 074704	3.9	157
454	Stable Metallic 1T-WS ₂ Nanoribbons Intercalated with Ammonia Ions: The Correlation between Structure and Electrical/Optical Properties. <i>Advanced Materials</i> , 2015 , 27, 4837-44	24	151
453	. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 11336-11342	3.8	150
452	Room-Temperature Ferromagnetism in Two-Dimensional FeSi Nanosheet with Enhanced Spin-Polarization Ratio. <i>Nano Letters</i> , 2017 , 17, 2771-2777	11.5	147
451	Effects of stacking order, layer number and external electric field on electronic structures of few-layer C ₂ N-h ₂ D. <i>Nanoscale</i> , 2015 , 7, 14062-70	7.7	147

450	Material Design for Photocatalytic Water Splitting from a Theoretical Perspective. <i>Advanced Materials</i> , 2018 , 30, e1802106	24	146
449	Site-specific photocatalytic splitting of methanol on TiO ₂ (110). <i>Chemical Science</i> , 2010 , 1, 575	9.4	143
448	Edge-Modified Phosphorene Nanoflake Heterojunctions as Highly Efficient Solar Cells. <i>Nano Letters</i> , 2016 , 16, 1675-82	11.5	142
447	A First-Principles Study on Electron Donor and Acceptor Molecules Adsorbed on Phosphorene. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 2871-2878	3.8	137
446	Adding two active silver atoms on Au nanoparticle. <i>Nano Letters</i> , 2015 , 15, 1281-7	11.5	137
445	Observation of photocatalytic dissociation of water on terminal Ti sites of TiO ₂ (110)-1 × 1 surface. <i>Journal of the American Chemical Society</i> , 2012 , 134, 9978-85	16.4	137
444	Molecular oxygen adsorption behaviors on the rutile TiO ₂ (110)-1 × 1 surface: an in situ study with low-temperature scanning tunneling microscopy. <i>Journal of the American Chemical Society</i> , 2011 , 133, 2002-9	16.4	135
443	Mechanism for negative differential resistance in molecular electronic devices: local orbital symmetry matching. <i>Physical Review Letters</i> , 2007 , 99, 146803	7.4	135
442	Rational Design of Cathode Structure for High Rate Performance Lithium-Sulfur Batteries. <i>Nano Letters</i> , 2015 , 15, 5443-8	11.5	131
441	Half-metallicity in hybrid BCN nanoribbons. <i>Journal of Chemical Physics</i> , 2008 , 129, 084712	3.9	129
440	CO ₂ Capture on h-BN Sheet with High Selectivity Controlled by External Electric Field. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 6912-6917	3.8	127
439	Negative differential-resistance device involving two C ₆₀ molecules. <i>Applied Physics Letters</i> , 2000 , 77, 3595-3597	3.4	125
438	Electronic Structure Engineering via On-Plane Chemical Functionalization: A Comparison Study on Two-Dimensional Polysilane and Graphane. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 16741-16746	3.8	122
437	Band-gap scaling of graphene nanohole superlattices. <i>Physical Review B</i> , 2009 , 80,	3.3	115
436	"Narrow" graphene nanoribbons made easier by partial hydrogenation. <i>Nano Letters</i> , 2009 , 9, 4025-30	11.5	115
435	Sub-nanometre control of the coherent interaction between a single molecule and a plasmonic nanocavity. <i>Nature Communications</i> , 2017 , 8, 15225	17.4	113
434	One-Nanometer-Thick PtNiRh Trimetallic Nanowires with Enhanced Oxygen Reduction Electrocatalysis in Acid Media: Integrating Multiple Advantages into One Catalyst. <i>Journal of the American Chemical Society</i> , 2018 , 140, 16159-16167	16.4	111
433	Porous silicene as a hydrogen purification membrane. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 5753-8	11.0	110

432	Semihydrogenated BN sheet: a promising visible-light driven photocatalyst for water splitting. <i>Scientific Reports</i> , 2013 , 3, 1858	4.9	109
431	New insight into the electronic shell of Au(38)(SR)(24): a superatomic molecule. <i>Nanoscale</i> , 2013 , 5, 1475-8	7.8	108
430	Unconventional p-d Hybridization Interaction in PtGa Ultrathin Nanowires Boosts Oxygen Reduction Electrocatalysis. <i>Journal of the American Chemical Society</i> , 2019 , 141, 18083-18090	16.4	107
429	Theoretical study of small two-dimensional gold clusters. <i>Physical Review B</i> , 2003 , 67,	3.3	106
428	Phosphorene: a two dimensional material with a highly negative Poisson's ratio. <i>Nanoscale</i> , 2017 , 9, 850-855	7.7	105
427	Tunable Schottky contacts in hybrid graphene-phosphorene nanocomposites. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 4756-4761	7.1	104
426	Electronic Structures and Magnetic Properties of GaN Sheets and Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 11390-11394	3.8	99
425	Superatom networks in thiolate-protected gold nanoparticles. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 9035-9	16.4	98
424	Single-molecule chemistry of metal phthalocyanine on noble metal surfaces. <i>Accounts of Chemical Research</i> , 2010 , 43, 954-62	24.3	98
423	Two-dimensional van der Waals heterojunctions for functional materials and devices. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 12289-12297	7.1	97
422	Crystal and Solution Photoluminescence of MAg ₂₄ (SR) ₁₈ (M = Ag/Pd/Pt/Au) Nanoclusters and Some Implications for the Photoluminescence Mechanisms. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 13848-13853	3.8	96
421	Two-Dimensional Phosphorus Porous Polymorphs with Tunable Band Gaps. <i>Journal of the American Chemical Society</i> , 2016 , 138, 7091-8	16.4	96
420	Half-Metallicity in Hybrid Graphene/Boron Nitride Nanoribbons with Dihydrogenated Edges. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 9442-9450	3.8	94
419	Mn ₂ C monolayer: a 2D antiferromagnetic metal with high Néel temperature and large spin-orbit coupling. <i>Nanoscale</i> , 2016 , 8, 12939-45	7.7	94
418	Single layer of MX ₂ (M = Ti, Zr; X = S, Se, Te): a new platform for nano-electronics and optics. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 18665-9	3.6	93
417	A Simple Molecular Design Strategy for Two-Dimensional Covalent Organic Framework Capable of Visible-Light-Driven Water Splitting. <i>Journal of the American Chemical Society</i> , 2020 , 142, 4508-4516	16.4	92
416	The g-C ₃ N ₄ /C ₂ N Nanocomposite: A g-C ₃ N ₄ -Based Water-Splitting Photocatalyst with Enhanced Energy Efficiency. <i>ChemPhysChem</i> , 2016 , 17, 2100-4	3.2	91
415	Understanding of Strain Effects in the Electrochemical Reduction of CO ₂ : Using Pd Nanostructures as an Ideal Platform. <i>Angewandte Chemie</i> , 2017 , 129, 3648-3652	3.6	89

4 ¹⁴	Effects of interlayer coupling and electric fields on the electronic structures of graphene and MoS ₂ heterobilayers. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 1776-1781	7.1	89
4 ¹³	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 3142-3146	3.8	88
4 ¹²	Direct hydrothermal synthesis of monoclinic VO ₂ (M) single-domain nanorods on large scale displaying magnetocaloric effect. <i>Journal of Materials Chemistry</i> , 2011 , 21, 4509		88
4 ¹¹	Half-metallicity in organic single porous sheets. <i>Journal of the American Chemical Society</i> , 2012 , 134, 5718-5721	16.4	87
4 ¹⁰	Hydrogen adsorption on zigzag (8,0) boron nitride nanotubes. <i>Journal of Chemical Physics</i> , 2004 , 121, 8481-5	3.9	87
4 ⁰⁹	Structures and magnetism of mono-palladium and mono-platinum doped Au ₂₅ (PET) ₁₈ nanoclusters. <i>Chemical Communications</i> , 2016 , 52, 9873-6	5.8	87
4 ⁰⁸	Highly confined water: two-dimensional ice, amorphous ice, and clathrate hydrates. <i>Accounts of Chemical Research</i> , 2014 , 47, 2505-13	24.3	85
4 ⁰⁷	Theoretical study of the molecular and electronic structure of methanol on a TiO ₂ (110) surface. <i>Physical Review B</i> , 2009 , 80,	3.3	84
4 ⁰⁶	Oxidation states of graphene: insights from computational spectroscopy. <i>Journal of Chemical Physics</i> , 2009 , 131, 244505	3.9	84
4 ⁰⁵	Structure of Graphene Oxide: Thermodynamics versus Kinetics. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 11991-11995	3.8	83
4 ⁰⁴	Helium separation via porous silicene based ultimate membrane. <i>Nanoscale</i> , 2013 , 5, 9062-6	7.7	82
4 ⁰³	Electronic and optical properties of graphene and graphitic ZnO nanocomposite structures. <i>Journal of Chemical Physics</i> , 2013 , 138, 124706	3.9	82
4 ⁰²	Icosahedral B ₁₂ -containing core-shell structures of B ₈₀ . <i>Chemical Communications</i> , 2010 , 46, 3878-80	5.8	82
4 ⁰¹	What are the adsorption sites for CO on the reduced TiO ₂ (110)-1 x 1 surface?. <i>Journal of the American Chemical Society</i> , 2009 , 131, 7958-9	16.4	81
4 ⁰⁰	Chiral selective tunneling induced negative differential resistance in zigzag graphene nanoribbon: A theoretical study. <i>Applied Physics Letters</i> , 2008 , 92, 133114	3.4	81
399	Lattice mismatch induced nonlinear growth of graphene. <i>Journal of the American Chemical Society</i> , 2012 , 134, 6045-51	16.4	80
398	Ferroelectric hexagonal and rhombic monolayer ice phases. <i>Chemical Science</i> , 2014 , 5, 1757-1764	9.4	79
397	Structural, electronic, and optical properties of hybrid silicene and graphene nanocomposite. <i>Journal of Chemical Physics</i> , 2013 , 139, 154704	3.9	79

396	Shape-Dependent Reducibility of Cuprous Oxide Nanocrystals. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 6676-6680	3.8	79
395	Azide Passivation of Black Phosphorus Nanosheets: Covalent Functionalization Affords Ambient Stability Enhancement. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 1479-1483	16.4	79
394	Two-dimensional van der Waals nanocomposites as Z-scheme type photocatalysts for hydrogen production from overall water splitting. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 18892-18898	13	78
393	Electronic and magnetic properties of V-doped anatase TiO ₂ from first principles. <i>Physical Review B</i> , 2006 , 74,	3.3	78
392	Band Structure Tuning of TiO ₂ for Enhanced Photoelectrochemical Water Splitting. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 7451-7457	3.8	77
391	Oxidation of a two-dimensional hexagonal boron nitride monolayer: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 5545-50	3.6	77
390	Hexagonal Cu ₂ SnS ₃ with metallic character: Another category of conducting sulfides. <i>Applied Physics Letters</i> , 2007 , 91, 143104	3.4	77
389	Direct Z-Scheme Water Splitting Photocatalyst Based on Two-Dimensional Van Der Waals Heterostructures. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 5419-5424	6.4	77
388	AlxC Monolayer Sheets: Two-Dimensional Networks with Planar Tetracoordinate Carbon and Potential Applications as Donor Materials in Solar Cell. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 2058-65	6.4	76
387	Electronic and Magnetic Properties of Metal Phthalocyanines on Au(111) Surface: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 13650-13655	3.8	75
386	Bimetal Doping in Nanoclusters: Synergistic or Counteractive?. <i>Chemistry of Materials</i> , 2016 , 28, 8240-8247	7	74
385	Design and control of electron transport properties of single molecules. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009 , 106, 15259-63	11.5	74
384	Room-temperature half-metallicity in La(Mn,Zn)AsO alloy via element substitutions. <i>Journal of the American Chemical Society</i> , 2014 , 136, 5664-9	16.4	73
383	First-principles study of two-dimensional van der Waals heterojunctions. <i>Computational Materials Science</i> , 2016 , 112, 518-526	3.2	72
382	Activating Edge Sites on Pd Catalysts for Selective Hydrogenation of Acetylene via Selective Ga ₂ O ₃ Decoration. <i>ACS Catalysis</i> , 2016 , 6, 3700-3707	13.1	72
381	Unusual Metallic Microporous Boron Nitride Networks. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3484-3488	6.4	69
380	Sub-nanometre resolution in single-molecule photoluminescence imaging. <i>Nature Photonics</i> , 2020 , 14, 693-699	33.9	69
379	Deformation-induced site selectivity for hydrogen adsorption on boron nitride nanotubes. <i>Physical Review B</i> , 2004 , 69,	3.3	68

378	Nonclassical behavior in the capacitance of a nanojunction. <i>Physical Review Letters</i> , 2001 , 86, 5321-4	7.4	68
377	Electrically driven single-photon emission from an isolated single molecule. <i>Nature Communications</i> , 2017 , 8, 580	17.4	67
376	Communication: Coalescence of carbon atoms on Cu (111) surface: Emergence of a stable bridging-metal structure motif. <i>Journal of Chemical Physics</i> , 2010 , 133, 071101	3.9	67
375	Porous Boron Nitride with Tunable Pore Size. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 393-8	6.4	66
374	Ultrahigh Infrared Photoresponse from Core-Shell Single-Domain-VO ₂ /V ₂ O ₅ Heterostructure in Nanobeam. <i>Advanced Functional Materials</i> , 2014 , 24, 1821-1830	15.6	66
373	Blockage of ultrafast and directional diffusion of Li atoms on phosphorene with intrinsic defects. <i>Nanoscale</i> , 2016 , 8, 4001-6	7.7	65
372	Exploration of Structures of Two-Dimensional Boron-Silicon Compounds with sp ² Silicon. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 561-7	6.4	64
371	Communication: new insight into electronic shells of metal clusters: analogues of simple molecules. <i>Journal of Chemical Physics</i> , 2013 , 138, 141101	3.9	64
370	Is mayenite without clathrated oxygen an inorganic electride?. <i>Angewandte Chemie - International Edition</i> , 2004 , 43, 6479-82	16.4	63
369	Structural and electronic properties of OsB ₂ : A hard metallic material. <i>Physical Review B</i> , 2006 , 74,	3.3	62
368	Kernel Tuning and Nonuniform Influence on Optical and Electrochemical Gaps of Bimetal Nanoclusters. <i>Journal of the American Chemical Society</i> , 2018 , 140, 3487-3490	16.4	61
367	Carbon dimers as the dominant feeding species in epitaxial growth and morphological phase transition of graphene on different Cu substrates. <i>Physical Review Letters</i> , 2015 , 114, 216102	7.4	61
366	MAGNETISM IN GRAPHENE SYSTEMS. <i>Nano</i> , 2008 , 03, 433-442	1.1	61
365	Graphene Thickness Control via Gas-Phase Dynamics in Chemical Vapor Deposition. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 10557-10562	3.8	59
364	Hydroxyls-induced oxygen activation on inert Au nanoparticles for low-temperature CO oxidation. <i>Journal of Catalysis</i> , 2011 , 277, 95-103	7.3	59
363	CO ₂ dissociation activated through electron attachment on the reduced rutile TiO ₂ (110)-1 \times 1 surface. <i>Physical Review B</i> , 2011 , 84,	3.3	59
362	Formation energies of topological defects in carbon nanotubes. <i>Physical Review B</i> , 2000 , 62, 12652-12655	3.3	59
361	Direct observation of single-molecule hydrogen-bond dynamics with single-bond resolution. <i>Nature Communications</i> , 2018 , 9, 807	17.4	56

- 360 What can a scanning tunneling microscope image do for the insulating alkanethiol molecules on Au(111) substrates?. *Journal of Chemical Physics*, **2002**, 117, 851-856 3.9 56
- 359 Single-layer cadmium chalcogenides: promising visible-light driven photocatalysts for water splitting. *Physical Chemistry Chemical Physics*, **2016**, 18, 17029-36 3.6 55
- 358 Highly-efficient heterojunction solar cells based on two-dimensional tellurene and transition metal dichalcogenides. *Journal of Materials Chemistry A*, **2019**, 7, 7430-7436 13 54
- 357 Excited states of the 3d transition metal monoxides. *Journal of Chemical Physics*, **2003**, 118, 9608-9613 3.9 54
- 356 β -Phosphorene: a new allotrope of phosphorene. *Physical Chemistry Chemical Physics*, **2017**, 19, 2402-2408 3.6 53
- 355 Two-dimensional multilayer M₂CO₂ (M = Sc, Zr, Hf) as photocatalysts for hydrogen production from water splitting: a first principles study. *Journal of Materials Chemistry A*, **2017**, 5, 24972-24980 13 53
- 354 Bipolar magnetic materials for electrical manipulation of spin-polarization orientation. *Physical Chemistry Chemical Physics*, **2013**, 15, 15793-801 3.6 52
- 353 Hydrogenated bilayer wurtzite SiC nanofilms: a two-dimensional bipolar magnetic semiconductor material. *Physical Chemistry Chemical Physics*, **2013**, 15, 497-503 3.6 52
- 352 Visually constructing the chemical structure of a single molecule by scanning Raman picoscopy. *National Science Review*, **2019**, 6, 1169-1175 10.8 51
- 351 Evidence of van Hove singularities in ordered grain boundaries of graphene. *Physical Review Letters*, **2014**, 112, 226802 7.4 51
- 350 Iron-phthalocyanine molecular junction with high spin filter efficiency and negative differential resistance. *Journal of Chemical Physics*, **2012**, 136, 064707 3.9 51
- 349 Atomic-Level Construction of Tensile-Strained PdFe Alloy Surface toward Highly Efficient Oxygen Reduction Electrocatalysis. *Nano Letters*, **2020**, 20, 1403-1409 11.5 50
- 348 Funnel hopping: Searching the cluster potential energy surface over the funnels. *Journal of Chemical Physics*, **2009**, 130, 214112 3.9 50
- 347 Transition metal atom embedded graphene for capturing CO: A first-principles study. *International Journal of Hydrogen Energy*, **2014**, 39, 20190-20196 6.7 49
- 346 Active hydrogen species on TiO₂ for photocatalytic H₂ production. *Physical Chemistry Chemical Physics*, **2014**, 16, 7051-7 3.6 49
- 345 Structure sensitivity of low-temperature NO decomposition on Au surfaces. *Journal of Catalysis*, **2013**, 304, 112-122 7.3 49
- 344 Formation and diffusion of oxygen-vacancy pairs on TiO₂(110)-(1x1). *Journal of Chemical Physics*, **2008**, 129, 044703 3.9 49
- 343 Quasi PdNi single-atom surface alloy catalyst enables hydrogenation of nitriles to secondary amines. *Nature Communications*, **2019**, 10, 4998 17.4 48

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