Shu-Ping Huang

List of Publications by Year
in descending order

119	8,291	117453 34	46693 89
papers	citations	h-index	g-index

127	127	127	7502
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Efficient blue organic light-emitting diodes employing thermally activated delayed fluorescence. Nature Photonics, 2014, 8, 326-332.	15.6	2,064
2	Design of Efficient Thermally Activated Delayed Fluorescence Materials for Pure Blue Organic Light Emitting Diodes. Journal of the American Chemical Society, 2012, 134, 14706-14709.	6.6	1,370
3	Anthraquinone-Based Intramolecular Charge-Transfer Compounds: Computational Molecular Design, Thermally Activated Delayed Fluorescence, and Highly Efficient Red Electroluminescence. Journal of the American Chemical Society, 2014, 136, 18070-18081.	6.6	822
4	Se2(B2O7):Â A New Type of Second-Order NLO Material. Journal of the American Chemical Society, 2006, 128, 7750-7751.	6.6	337
5	Computational Prediction for Singlet- and Triplet-Transition Energies of Charge-Transfer Compounds. Journal of Chemical Theory and Computation, 2013, 9, 3872-3877.	2.3	312
6	Triplet Exciton Confinement in Green Organic Lightâ€Emitting Diodes Containing Luminescent Chargeâ€Transfer Cu(I) Complexes. Advanced Functional Materials, 2012, 22, 2327-2336.	7.8	279
7	High-efficiency deep-blue organic light-emitting diodes based on a thermally activated delayed fluorescence emitter. Journal of Materials Chemistry C, 2014, 2, 421-424.	2.7	259
8	Bismuth Nanoparticle@Carbon Composite Anodes for Ultralong Cycle Life and Highâ€Rate Sodiumâ€Ion Batteries. Advanced Materials, 2019, 31, e1904771.	11.1	201
9	Explorations of New Types of Secondâ€Order Nonlinear Optical Materials in Cd(Zn)â€V^Vâ€Te^{IV}â€O Systems. Chemistry - A European Journal, 2008, 14, 1972-1981.	1.7	103
10	Hierarchical spheres constructed by ultrathin VS₂ nanosheets for sodium-ion batteries. Journal of Materials Chemistry A, 2019, 7, 3691-3696.	5.2	94
11	KMBP₂O₈ (M = Sr, Ba): A New Kind of Noncentrosymmetry Borophosphate with the Three-Dimensional Diamond-like Framework. Inorganic Chemistry, 2009, 48, 6623-6629.	1.9	93
12	Moleculeâ€“substrate interaction channels of metal-phthalocyanines on graphene on Ni(111) surface. Journal of Chemical Physics, 2011, 134, 094705.	1.2	74
13	MnSb₂S₄ Monolayer as an Anode Material for Metal-Ion Batteries. Chemistry of Materials, 2018, 30, 3208-3214.	3.2	74
14	1T-MoS2 monolayer as a promising anode material for (Li/Na/Mg)-ion batteries. Applied Surface Science, 2022, 584, 152537.	3.1	66
15	Hierarchical Composite of Roseâ€Like VS₂@S/Nâ€Doped Carbon with Expanded (001) Planes for Superior Liâ€Ion Storage. Small, 2019, 15, e1903904.	5.2	64
16	Safe, Lowâ€Cost, Fastâ€Kinetics and Lowâ€Strain Inorganicâ€Openâ€Framework Anode for Potassiumâ€Ion Batteries. Angewandte Chemie - International Edition, 2019, 58, 16474-16479.	7.2	56
17	Y-doped Li₈ZrO₆: A Li-Ion Battery Cathode Material with High Capacity. Journal of the American Chemical Society, 2015, 137, 10992-11003.	6.6	54
18	Rational Design of Hierarchical SnS₂ Microspheres with S Vacancy for Enhanced Sodium Storage Performance. ACS Sustainable Chemistry and Engineering, 2020, 8, 9519-9525.	3.2	52

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19	Density Functional Theory Study of Single-Atom V, Nb, and Ta Catalysts on Graphene and Carbon Nitride for Selective Nitrogen Reduction. ACS Applied Nano Materials, 2020, 3, 5149-5159.	2.4	51
20	First-principles study: size-dependent optical properties for semiconducting silicon carbide nanotubes. Optics Express, 2007, 15, 10947.	1.7	49
21	Whether Corrugated or Planar Vacancy Graphene-like Carbon Nitride (g-C₃N₄) Is More Effective for Nitrogen Reduction Reaction?. Journal of Physical Chemistry C, 2019, 123, 17296-17305.	1.5	46
22	Sulfur-Doped Anatase TiO₂ as an Anode for High-Performance Sodium-Ion Batteries. ACS Applied Energy Materials, 2019, 2, 3791-3797.	2.5	46
23	Photoinduced rearrangement of vinyl tosylates to Î²-ketosulfones. Green Chemistry, 2017, 19, 3530-3534.	4.6	45
24	Theoretical studies of SiC van der Waals heterostructures as anodes of Li-ion batteries. Applied Surface Science, 2021, 563, 150269.	3.1	43
25	Starburst Triarylamine Donor-Based Metal-Free Photosensitizers for Photocatalytic Hydrogen Production from Water. Organic Letters, 2017, 19, 1048-1051.	2.4	42
26	Mechanism of electrochemical lithiation of a metal-organic framework without redox-active nodes. Journal of Chemical Physics, 2016, 144, 194702.	1.2	41
27	Cercosporin-bioinspired selective photooxidation reactions under mild conditions. Green Chemistry, 2019, 21, 6073-6081.	4.6	41
28	DFT study of the mechanism for methane hydroxylation by soluble methane monooxygenase (sMMO): effects of oxidation state, spin state, and coordination number. Dalton Transactions, 2013, 42, 1011-1023.	1.6	40
29	Perylenequinonoid-Catalyzed [4 + 1] and [4 + 2] Annulations of Azoalkenes: Photocatalytic Access to 1,2,3-Thiadiazole/1,4,5,6-Tetrahydropyridazine Derivatives. Journal of Organic Chemistry, 2019, 84, 7711-7721.	1.7	40
30	Perylenequinonoid-catalyzed photoredox activation for the direct arylation of (het)arenes with sunlight. Organic and Biomolecular Chemistry, 2019, 17, 4364-4369.	1.5	40
31	Theoretical calculations of structures and properties of one-dimensional silicon-based nanomaterials: Particularities and peculiarities of silicon and silicon-containing nanowires and nanotubes. Coordination Chemistry Reviews, 2009, 253, 2935-2958.	9.5	38
32	Density functional theoretical determinations of electronic and optical properties of nanowires and bulks for CdS and CdSe. Applied Physics Letters, 2007, 90, 031904.	1.5	37
33	First-principles modeling of nonlinear optical properties of C3N4 polymorphs. Applied Physics Letters, 2006, 89, 261117.	1.5	36
34	Metalâ€“organic framework-derived hollow structure CoS₂/nitrogen-doped carbon spheres for high-performance lithium/sodium ion batteries. Chemical Communications, 2020, 56, 3951-3954.	2.2	35
35	Tuning Electronic Structures of ZnO Nanowires by Surface Functionalization: A First-Principles Study. Journal of Physical Chemistry C, 2010, 114, 8861-8866.	1.5	34
36	Reversible conversion reaction of GeO₂ boosts lithium-ion storage via Fe doping. Journal of Materials Chemistry A, 2019, 7, 4574-4580.	5.2	34

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37	Electronic properties of red and black phosphorous and their potential application as photocatalysts. RSC Advances, 2016, 6, 80872-80884.	1.7	33
38	Phthalocyanine and Metal Phthalocyanines Adsorbed on Graphene: A Density Functional Study. Journal of Physical Chemistry C, 2019, 123, 16614-16620.	1.5	33
39	N-Doped carbon encapsulating Bi nanoparticles derived from metalâ€“organic frameworks for high-performance sodium-ion batteries. Journal of Materials Chemistry A, 2021, 9, 22048-22055.	5.2	33
40	What Is the Best Size of Subnanometer Copper Clusters for CO₂ Conversion to Methanol at Cu/TiO₂ Interfaces? A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 24118-24132.	1.5	32
41	Zn[Htma][ddm]: An Interesting Three-Dimensional Chiral Nonlinear Optical-Active Zinc-Trimesate Framework. Crystal Growth and Design, 2010, 10, 930-936.	1.4	31
42	New bithiazole-functionalized organic photosensitizers for dye-sensitized solar cells. Dyes and Pigments, 2013, 96, 516-524.	2.0	31
43	Computational prediction for oxidation and reduction potentials of organic molecules used in organic light-emitting diodes. Organic Electronics, 2019, 64, 216-222.	1.4	31
44	Transition-Metal-Doped M-Li₈ZrO₆ (M = Mn, Fe, Co, Ni, Cu, Ce) as High-Specific-Capacity Li-Ion Battery Cathode Materials: Synthesis, Electrochemistry, and Quantum Mechanical Characterization. Chemistry of Materials, 2016, 28, 746-755.	3.2	30
45	Synthesis, structure, and photophysics of copper(<scp>i</scp>) triphenylphosphine complexes with functionalized 3-(2â€²-pyrimidinyl)-1,2,4-triazole ligands. Dalton Transactions, 2017, 46, 13077-13087.	1.6	30
46	Panchromatic Sensitization with Zn II Porphyrinâ€Based Photosensitizers for Lightâ€Driven Hydrogen Production. ChemSusChem, 2018, 11, 2517-2528.	3.6	30
47	Nanocomposite of Mo₂N Quantum Dots@MoO₃@Nitrogen-Doped Carbon as a High-Performance Anode for Lithium-Ion Batteries. ACS Sustainable Chemistry and Engineering, 2019, 7, 10198-10206.	3.2	30
48	Effects of doping high-valence transition metal (V, Nb and Zr) ions on the structure and electrochemical performance of LIB cathode material LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂. Physical Chemistry Chemical Physics, 2021, 23, 11528-11537.	1.3	29
49	Excited State Dynamics of Ru₁₀ Cluster Interfacing Anatase TiO₂(101) Surface and Liquid Water. Journal of Physical Chemistry Letters, 2014, 5, 2823-2829.	2.1	28
50	Blue-AsP monolayer as a promising anode material for lithium- and sodium-ion batteries: a DFT study. Physical Chemistry Chemical Physics, 2021, 23, 5143-5151.	1.3	28
51	Charge Transfer, Luminescence, and Phonon Bottleneck in TiO₂ Nanowires Computed by Eigenvectors of Liouville Superoperator. Journal of Chemical Theory and Computation, 2014, 10, 3996-4005.	2.3	26
52	A theoretical investigation of hyperpolarizability for small GanAsm (n+m=4â€“10) clusters. Journal of Chemical Physics, 2006, 124, 094302.	1.2	24
53	A New Candidate in Polyanionic Compounds for a Potassium-Ion Battery Cathode: KTiOPO₄. Journal of Physical Chemistry Letters, 2021, 12, 2721-2726.	2.1	23
54	Easily fabricated HARCP/HAp photocatalyst for efficient and fast removal of tetracycline under natural sunlight. Chemical Engineering Journal, 2021, 412, 128620.	6.6	23

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55	SOSâˆ¥TDDFT study on the dynamic third-order nonlinear optical properties of aniline oligomers based on the optimized configurations. Polymer, 2006, 47, 1749-1754.	1.8	22
56	BC₂N/Graphene Heterostructure as a Promising Anode Material for Rechargeable Li-Ion Batteries by Density Functional Calculations. Journal of Physical Chemistry C, 2019, 123, 30809-30818.	1.5	22
57	Different Atomic Terminations Affect the Photocatalytic Nitrogen Fixation of Bismuth Oxybromide: A First Principles Study. Chemistry - an Asian Journal, 2018, 13, 799-808.	1.7	21
58	UiO-66 Metalâ€“Organic Framework as an Anode for a Potassium-Ion Battery: Quantum Mechanical Analysis. Journal of Physical Chemistry C, 2021, 125, 9679-9687.	1.5	21
59	Non-collinear spin DFT for lanthanide ions in doped hexagonal NaYF₄. Molecular Physics, 2014, 112, 546-556.	0.8	19
60	Cercosporin-bioinspired photoreductive activation of aryl halides under mild conditions. Journal of Catalysis, 2019, 380, 1-8.	3.1	19
61	Large-scale preparation of heterometallic chalcogenide MnSb₂S₄monolayer nanosheets with a high visible-light photocatalytic activity for H₂evolution. Chemical Communications, 2016, 52, 13381-13384.	2.2	18
62	Localizing Holes as Polarons and Predicting Band Gaps, Defect Levels, and Delithiation Energies of Solid-State Materials with a Local Exchange-Correlation Functional. Journal of Physical Chemistry C, 2017, 121, 23955-23963.	1.5	18
63	Electronic structure and hot carrier relaxation in âŸ¨001âŸ© anatase TiO₂nanowire. Molecular Physics, 2014, 112, 539-545.	0.8	17
64	From Molecule to Bulk Material: Optical Properties of Hydrogen-Bonded Dimers [C12H12N4O2AgPF6]2 and [C28H28N6O3AgPF6]2 Depend on the Arrangement of the Oxime Moieties. Chemistry - A European Journal, 2007, 13, 5151-5159.	1.7	16
65	Synthesis, crystal and band structures, and properties of a new supramolecular complex (Hg2As)2(CdI4). Journal of Solid State Chemistry, 2007, 180, 805-811.	1.4	16
66	Crystal and band structure of K2AlTi(PO4)3 with the langbeinite-type structure. Journal of Alloys and Compounds, 2009, 477, 795-799.	2.8	16
67	Indium selenide monolayer: a two-dimensional material with strong second harmonic generation. CrystEngComm, 2018, 20, 2573-2582.	1.3	16
68	Development of Strong Visibleâ€Lightâ€Absorbing Cyclometalated Iridium(III) Complexes for Robust and Efficient Lightâ€Driven Hydrogen Production. Chemistry - A European Journal, 2022, 28, .	1.7	16
69	Oligothiopheneâ€Bridged Bis(arylene ethynylene) Small Molecules for Solutionâ€Processible Organic Solar Cells with High Openâ€Circuit Voltage. Chemistry - an Asian Journal, 2013, 8, 1892-1900.	1.7	15
70	Exploring the potentials of Ti₃N₂ and Ti₃N₂X₂ (X = O, F, OH) monolayers as anodes for Li or non-Li ion batteries from first-principles calculations. RSC Advances, 2019, 9, 40340-40347.	1.7	15
71	Defective BC₂N as an Anode Material with Improved Performance for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2021, 125, 4946-4954.	1.5	15
72	First-principles study of the elastic and optical properties of the pseudocubic Si₃As₄, Ge₃As₄and Sn₃As₄. Journal of Physics Condensed Matter, 2007, 19, 496215.	0.7	14

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73	Conduction and Surface Effects in Cathode Materials: Li₈ZrO₆ and Doped Li₈ZrO₆. Journal of Physical Chemistry C, 2016, 120, 9637-9649.	1.5	14
74	Carbon-based dots for the electrochemical production of hydrogen peroxide. Chemical Communications, 2020, 56, 7609-7612.	2.2	14
75	Syntheses, crystal structures, energy bands, and optical characterizations of Na5Ln(MoO4)4 (Ln=Gd,) Tj ETQq1 1 0.784314 rgBT /Ove	1.8	13
76	Ab Initio Study on Thermal and Chemical Stabilities of Silicon Monoxide Clusters. Journal of Physical Chemistry C, 2009, 113, 12736-12741.	1.5	13
77	Lithiation Abilities of SiC Bulks and Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 7031-7038.	1.5	13
78	Thiourea-based polyimide/RGO composite cathode: A comprehensive study of storage mechanism with alkali metal ions. Science China Materials, 2020, 63, 1929-1938.	3.5	13
79	First-principles calculations of band structures and dynamic optical properties of CsCdBr3 and RbCdI3â^™H2O crystals. Journal of Applied Physics, 2006, 99, 013516.	1.1	12
80	Syntheses, crystal structures, and characterizations of LiM(PO3)4 (M = Y, Dy). Journal of Molecular Structure, 2008, 892, 8-12.	1.8	12
81	A periodic density functional theory study on the effects of halides encapsulated in SiC nanotubes. Journal of Chemical Physics, 2008, 129, 174108.	1.2	12
82	Why does F-doping enhance the photocatalytic water-splitting performance of mBiVO₄? â€“ a density functional theory study. New Journal of Chemistry, 2017, 41, 1094-1102.	1.4	12
83	Toward an Accurate Description of Thermally Activated Delayed Fluorescence: Equal Importance of Electronic and Geometric Factors. Journal of Physical Chemistry C, 2019, 123, 13869-13876.	1.5	11
84	In Situ Confined Co5Ge3 Alloy Nanoparticles in Nitrogen-Doped Carbon Nanotubes for Boosting Lithium Storage. ACS Applied Materials & Interfaces, 2020, 12, 46247-46253.	4.0	11
85	Anionic Oxygen Redox in the High-Lithium Material Li₈SnO₆. Chemistry of Materials, 2021, 33, 834-844.	3.2	10
86	SIZE EFFECT OF ENCASED ATOM ON ABSORPTION AND NONLINEAR OPTICAL PROPERTIES OF EMBEDDED METALLOFULLERENES M@C82 (M = Sc, Y, La). Journal of Theoretical and Computational Chemistry, 2008, 07, 737-749.	1.8	9
87	Electronic and Vibrational Properties of Stable Isomers of (SiO)_n^(0,Â±) (n = 2â€“7) Clusters. Journal of Physical Chemistry A, 2014, 118, 8893-8900.	1.1	9
88	Tailoring the Linear and Second-Order Nonlinear Optical Responses of the Titanium-MIL-125 Metalâ€“Organic Framework through Ligand Functionalization: A First Principles Study. Journal of Physical Chemistry C, 2019, 123, 653-664.	1.5	9
89	Investigation of Ordered TiMC and TiMCT₂ (M = Cr and Mo; T = O and S) MXenes as High-Performance Anode Materials for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2022, 126, 5283-5291.	1.5	9
90	Highly efficient decontamination of tetracycline and pathogen by a natural product-derived Emodin/HAp photocatalyst. Chemosphere, 2022, 305, 135401.	4.2	9

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91	Modeling of configurations and third-order nonlinear optical properties of methyl silsesquioxanes. Journal of Chemical Physics, 2005, 122, 204709.	1.2	8
92	Theoretical Study of Two-Photon Absorption in Donorâ"Acceptor Chromophores Tetraalkylammonium Halide/Carbon Tetrabromide. Journal of Physical Chemistry A, 2006, 110, 10330-10335.	1.1	7
93	Electronic Origin for Enhanced Nonlinear Optical Response of Complexes from Tetraalkylammonium Halide and Carbon Tetrabromide: Electrostatic Potentials of Intermolecular Donorâ€"Acceptor Dyads. Chemistry - A European Journal, 2006, 12, 6880-6887.	1.7	7
94	Surface Passivationâ€Induced Strong Ferromagnetism of Zinc Oxide Nanowires. Chemistry - A European Journal, 2010, 16, 13072-13076.	1.7	7
95	Theoretical study on Y-doped Na₂ZrO₃ as a high-capacity Na-rich cathode material based on anionic redox. Physical Chemistry Chemical Physics, 2022, 24, 16183-16192.	1.3	7
96	Molecular Engineering of Robust Starburst-Based Organic Photosensitizers for Highly Efficient Photocatalytic Hydrogen Generation from Water. Chemistry of Materials, 2022, 34, 5522-5534.	3.2	7
97	Theoretical insights into the thermal reduction of N2 to NH3 over a single metal atom incorporated nitrogen-doped graphene. Journal of Chemical Physics, 2021, 154, 054703.	1.2	6
98	Energy-Transfer-Mediated Photocatalysis by a Bioinspired Organic Perylenephotosensitizer HiBRCP. Journal of Organic Chemistry, 2021, 86, 15284-15297.	1.7	6
99	Validation of Density Functional Theory Methods for Predicting the Optical Properties of Cu-Based Multinary Chalcogenide Semiconductors. Journal of Physical Chemistry C, 2022, 126, 4684-4697.	1.5	6
100	DFT investigations of KTiOPO4Mx (M = K, Na, and Li) anodes for alkali-ion battery. Journal of Chemical Physics, 2022, 156, .	1.2	6
101	Ab initiocharacterization of the electronic and optical properties of a new IR nonlinear optical crystal: K3V5O14. Journal of Physics Condensed Matter, 2006, 18, 5535-5544.	0.7	5
102	Effect of Cage Charges on Multiphoton Absorptions: First-Principles Study on Metallofullerenes Sc₂C₂@C₆₈ and Sc₃N@C₆₈. Journal of Physical Chemistry A, 2009, 113, 5966-5971.	1.1	5
103	Dynamics of charge at water-to-semiconductor interface: Case study of wet [0 0 1] anatase TiO2 nanowire. Chemical Physics, 2016, 481, 184-190.	0.9	5
104	Discovery and characterization of a novel perylenephotoreductant for the activation of aryl halides. Journal of Catalysis, 2021, 399, 111-120.	3.1	5
105	Understanding the Role of Various Dopant Metals (Sb, Sn, Ga, Ge, and V) in the Structural and Electrochemical Performances of LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂. Journal of Physical Chemistry C, 2021, 125, 19600-19608.	1.5	5
106	Selfâ€Optimizing Effect in Lithium Storage of GeO₂ Induced by Heterointerface Regulation. Small, 2022, 18, e2106067.	5.2	5
107	Potassium Storage Performance of UiO-66 Derivatives from First Principles Calculations. Journal of Physical Chemistry C, 2022, 126, 4286-4295.	1.5	5
108	Graphene-enhanced intermolecular interaction at interface between copper- and cobalt-phthalocyanines. Journal of Chemical Physics, 2015, 143, 134706.	1.2	4

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109	Effective Electrochemical Charge Storage in the High-Lithium Compound Li₈ZrO₆. ACS Applied Energy Materials, 2019, 2, 1274-1287.	2.5	4
110	Theoretical Insights into Synergistic Effects at Cu/TiC Interfaces for Promoting CO2 Activation. ACS Omega, 2021, 6, 27259-27270.	1.6	4
111	Band-gap control optical Kerr effect and light self-focusing of semiconducting materials CdxHg1â^'xGa2S4. Applied Physics Letters, 2005, 87, 141905.	1.5	3
112	Possible Reaction Paths of Small Silicon Clusters with Oxygen Explored with Density Functional Theory. Journal of Physical Chemistry C, 2010, 114, 13196-13203.	1.5	3
113	Anatase TiO2 Nanowires, Thin Films, and Surfaces: Ab initio Studies of Electronic Properties and Non-adiabatic Excited State Dynamics. Materials Research Society Symposia Proceedings, 2014, 1659, 129-134.	0.1	3
114	Carborane bridged ferrocenyl conjugated molecules: synthesis, structure, electrochemistry and photophysical properties. New Journal of Chemistry, 2020, 44, 7569-7576.	1.4	3
115	Length dependence of linear and nonlinear optical properties of finite-length BN(5,0) nanotube. Chinese Physics B, 2006, 15, 1563-1569.	1.3	2
116	First-Principles Determinations and Investigations of the Electronic Absorption and Third-Order Polarizability Spectra of Electron Donorâ^'Acceptor Chromophores Tetraalkylammonium Halide/Carbon Tetrabromide. Journal of Physical Chemistry A, 2007, 111, 9249-9254.	1.1	2
117	Li₈MnO₆: A Novel Cathode Material with Only Anionic Redox. ACS Applied Materials & Interfaces, 2022, 14, 29832-29843.	4.0	2
118	Theoretical Design of Layered AlGaS3 as a New Nonlinear Optical Material with a Strong Second Harmonic Generation Response. Crystal Growth and Design, 2019, 19, 1632-1639.	1.4	1
119	Electronic Structure and Excited State Dynamics of TiO₂Nanowires. ACS Symposium Series, 2019, , 23-46.	0.5	0