# Yun Wang

# List of Publications by Year in Descending Order

Source: https://exaly.com/author-pdf/1734056/yun-wang-publications-by-year.pdf

Version: 2024-04-10

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

 195
 10,629
 51
 99

 papers
 citations
 h-index
 g-index

 206
 12,747
 9.6
 6.39

 ext. papers
 ext. citations
 avg, IF
 L-index

| #   | Paper   | IF   | Citations |
|-----|---|------|-----------|
| 195 | Photocatalytic Hydrogen Production <b>2022</b> , 415-483  |      |           |
| 194 | TMN4 complex embedded graphene as efficient and selective electrocatalysts for chlorine evolution reactions. <i>Journal of Electroanalytical Chemistry</i> , <b>2022</b> , 907, 116071  | 4.1  | 4         |
| 193 | Theoretical understanding of electronic and mechanical properties of 1TN ransition metal dichalcogenide crystals <i>Beilstein Journal of Nanotechnology</i> , <b>2022</b> , 13, 160-171   | 3    | 1         |
| 192 | Highly efficient removal of Cr(VI) by hexapod-like pyrite nanosheet clusters. <i>Journal of Hazardous Materials</i> , <b>2022</b> , 424, 127504   | 12.8 | 2         |
| 191 | Insightful understanding of charge transfer processes in metalated phthalocyanines <i>Physical Chemistry Chemical Physics</i> , <b>2022</b> , 24, 7635-7641   | 3.6  |           |
| 190 | EArsenene Monolayer: A Promising Electrocatalyst for Anodic Chlorine Evolution Reaction.<br>Catalysts, <b>2022</b> , 12, 296  | 4    | O         |
| 189 | Operando Converting BiOCl into BiO(CO)Cl for Efficient Electrocatalytic Reduction of Carbon Dioxide to Formate <i>Nano-Micro Letters</i> , <b>2022</b> , 14, 121  | 19.5 | O         |
| 188 | The Role of Steps on Silver Nanoparticles in Electrocatalytic Oxygen Reduction. <i>Catalysts</i> , <b>2022</b> , 12, 576  | 4    | 1         |
| 187 | Rational design of metal oxide catalysts for electrocatalytic water splitting. <i>Nanoscale</i> , <b>2021</b> ,   | 7.7  | 7         |
| 186 | Reinvestigating oxygen adsorption on Ag(111) by using strongly constrained and appropriately normed semi-local density functional with the revised Vydrov van Voorhis van der Waals force correction <i>Journal of Chemical Physics</i> , <b>2021</b> , 155, 234704 | 3.9  | 2         |
| 185 | Engineering Crystallinity and Oxygen Vacancies of Co(II) Oxide Nanosheets for High Performance and Robust Rechargeable ZnAir Batteries. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2101239  | 15.6 | 52        |
| 184 | Grey hematite photoanodes decrease the onset potential in photoelectrochemical water oxidation. <i>Science Bulletin</i> , <b>2021</b> , 66, 1013-1021   | 10.6 | 4         |
| 183 | Mechanical properties of lateral transition metal dichalcogenide heterostructures. <i>Frontiers of Physics</i> , <b>2021</b> , 16, 1  | 3.7  | 5         |
| 182 | Numerical Simulation of Electrified Solid[liquid Interfaces <b>2021</b> , 1-18  |      |           |
| 181 | Scalable and controllable fabrication of CNTs improved yolk-shelled Si anodes with advanced in operando mechanical quantification. <i>Energy and Environmental Science</i> , <b>2021</b> , 14, 3502-3509  | 35.4 | 14        |
| 180 | Theory <b>E</b> xperiment Gap <b>2021</b> , 1-14  |      | 1         |
| 179 | Anchoring Single Copper Atoms to Microporous Carbon Spheres as High-Performance Electrocatalyst for Oxygen Reduction Reaction. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2104864   | 15.6 | 19        |

# (2020-2021)

| 178 | Oxygen-terminated M4X3 MXenes with superior mechanical strength. <i>Mechanics of Materials</i> , <b>2021</b> , 160, 103957  | 3.3  | 3   |  |
|-----|---|------|-----|--|
| 177 | Cesium-doped Ti3C2Tx MXene for efficient and thermally stable perovskite solar cells. <i>Cell Reports Physical Science</i> , <b>2021</b> , 2, 100598  | 6.1  | 6   |  |
| 176 | Stone-Wales defect-rich carbon-supported dual-metal single atom sites for Zn-air batteries. <i>Nano Energy</i> , <b>2021</b> , 90, 106488   | 17.1 | 9   |  |
| 175 | Multiscale numerical simulation of in-plane mechanical properties of two-dimensional monolayers <i>RSC Advances</i> , <b>2021</b> , 11, 20232-20247   | 3.7  | 3   |  |
| 174 | Theoretical understanding of the properties of stepped iron surfaces with van der Waals interaction corrections. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 2649-2657                                       | 3.6  | 2   |  |
| 173 | Reliably Probing the Conductance of a Molecule in a Cavity via van der Waals Contacts. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 16143-16148  | 3.8  | 7   |  |
| 172 | Aluminium-induced component engineering of mesoporous composite materials for low-temperature NH3-SCR. <i>Communications Chemistry</i> , <b>2020</b> , 3,   | 6.3  | 5   |  |
| 171 | Lattice-compressed and N-doped Co nanoparticles to boost oxygen reduction reaction for zinc-air batteries. <i>Applied Surface Science</i> , <b>2020</b> , 525, 146491   | 6.7  | 9   |  |
| 170 | Effect of Structural Phases on Mechanical Properties of Molybdenum Disulfide. <i>ACS Omega</i> , <b>2020</b> , 5, 5994-6002   | 3.9  | 21  |  |
| 169 | How Cobalt and Iron Doping Determine the Oxygen Evolution Electrocatalytic Activity of NiOOH. <i>Cell Reports Physical Science</i> , <b>2020</b> , 1, 100077  | 6.1  | 15  |  |
| 168 | Phosphorus and Sulfur Co-Doped Cobaltous Oxide Synthesized by an Inorganic-Salt-Assisted Method: Reaction Mechanism and Electrocatalytic Application. <i>ChemPlusChem</i> , <b>2020</b> , 85, 1602-1611                         | 2.8  | 2   |  |
| 167 | Surface oxidized two-dimensional antimonene nanosheets for electrochemical ammonia synthesis under ambient conditions. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 4735-4739                                     | 13   | 37  |  |
| 166 | Ligand-assisted cation-exchange engineering for high-efficiency colloidal Cs1NFAxPbI3 quantum dot solar cells with reduced phase segregation. <i>Nature Energy</i> , <b>2020</b> , 5, 79-88                                     | 62.3 | 237 |  |
| 165 | Bottom-Up Fabrication of a Sandwich-Like Carbon/Graphene Heterostructure with Built-In FeNC Dopants as Non-Noble Electrocatalyst for Oxygen Reduction Reaction. <i>Chemistry - an Asian Journal</i> , <b>2020</b> , 15, 432-439 | 4.5  | 9   |  |
| 164 | An efficient defect engineering strategy to enhance catalytic performances of CoO nanorods for CO oxidation. <i>Journal of Hazardous Materials</i> , <b>2020</b> , 394, 122540  | 12.8 | 16  |  |
| 163 | An inverted Bil3/PCBM binary quasi-bulk heterojunction solar cell with a power conversion efficiency of 1.50%. <i>Nano Energy</i> , <b>2020</b> , 73, 104799  | 17.1 | 11  |  |
| 162 | Super strong 2D titanium carbide MXene-based materials: a theoretical prediction. <i>Journal of Physics Condensed Matter</i> , <b>2020</b> , 32, 11LT01   | 1.8  | 8   |  |
| 161 | Effects of compositional engineering and surface passivation on the properties of halide perovskites: a theoretical understanding. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 19718-19724                   | 3.6  | 4   |  |

| 160 | Selective Growth of High-Density Anatase {101} Twin Boundaries on High-Energy {001} Facets.<br>Small Structures, <b>2020</b> , 1, 2000025   | 8.7  | 10  |
|-----|---|------|-----|
| 159 | Surface chelation of cesium halide perovskite by dithiocarbamate for efficient and stable solar cells. <i>Nature Communications</i> , <b>2020</b> , 11, 4237  | 17.4 | 62  |
| 158 | Coexisting Single-Atomic Fe and Ni Sites on Hierarchically Ordered Porous Carbon as a Highly Efficient ORR Electrocatalyst. <i>Advanced Materials</i> , <b>2020</b> , 32, e2004670  | 24   | 170 |
| 157 | Theoretical Understanding of Electrocatalytic Hydrogen Production Performance by Low-Dimensional Metal-Organic Frameworks on the Basis of Resonant Charge-Transfer Mechanisms. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 6955-6961 | 6.4  | 4   |
| 156 | Construction of a sp3/sp2 Carbon Interface in 3D N-Doped Nanocarbons for the Oxygen Reduction Reaction. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 15233-15241   | 3.6  | 30  |
| 155 | Construction of a sp /sp Carbon Interface in 3D N-Doped Nanocarbons for the Oxygen Reduction Reaction. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 15089-15097   | 16.4 | 110 |
| 154 | General strategy toward hexagonal ring-like layered double hydroxides and their application for asymmetric supercapacitors. <i>Chemical Engineering Journal</i> , <b>2019</b> , 375, 121926   | 14.7 | 32  |
| 153 | Molecular discovery of half-metallic one-dimensional metal-organic framework. <i>Journal of Applied Physics</i> , <b>2019</b> , 125, 142906   | 2.5  | 5   |
| 152 | Superior triethylamine detection at room temperature by {-112} faceted WO gas sensor. <i>Journal of Hazardous Materials</i> , <b>2019</b> , 380, 120876   | 12.8 | 48  |
| 151 | Integrated N-Co/Carbon Nanofiber Cathode for Highly Efficient Zinc-Air Batteries. <i>ACS Applied Materials &amp; Amp; Interfaces</i> , <b>2019</b> , 11, 29708-29717  | 9.5  | 23  |
| 150 | Heteroatom-Mediated Interactions between Ruthenium Single Atoms and an MXene Support for Efficient Hydrogen Evolution. <i>Advanced Materials</i> , <b>2019</b> , 31, e1903841   | 24   | 197 |
| 149 | Large expert-curated database for benchmarking document similarity detection in biomedical literature search. <i>Database: the Journal of Biological Databases and Curation</i> , <b>2019</b> , 2019,   | 5    | 4   |
| 148 | Overall electrochemical splitting of water at the heterogeneous interface of nickel and iron oxide. <i>Nature Communications</i> , <b>2019</b> , 10, 5599   | 17.4 | 246 |
| 147 | Sulfur-doped cobalt oxide nanowires as efficient electrocatalysts for iodine reduction reaction.<br>Journal of Alloys and Compounds, <b>2019</b> , 772, 80-91   | 5.7  | 10  |
| 146 | 2DØD Heterostructured UNiMOF/g-C3N4 for Enhanced Photocatalytic H2 Production under Visible-Light Irradiation. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2019</b> , 7, 2492-2499  | 8.3  | 52  |
| 145 | Rapid-Heating-Triggered in Situ Solid-State Transformation of Amorphous TiO2 Nanotubes into Well-Defined Anatase Nanocrystals. <i>Crystal Growth and Design</i> , <b>2019</b> , 19, 1086-1094   | 3.5  | 3   |
| 144 | A Gradient Heterostructure Based on Tolerance Factor in High-Performance Perovskite Solar Cells with 0.84 Fill Factor. <i>Advanced Materials</i> , <b>2019</b> , 31, e1804217   | 24   | 70  |
| 143 | Wet-chemistry grafted active pyridinic nitrogen sites on holey graphene edges as high performance ORR electrocatalyst for Zn-Air[batteries. <i>Materials Today Energy</i> , <b>2019</b> , 11, 24-29   | 7    | 16  |

#### (2018-2019)

| 142                             | Correlating electrocatalytic activities with sulfur species on sulfur-doped cobalt oxide. <i>Materials Letters</i> , <b>2019</b> , 236, 614-617  | 3.3                        | 1   |
|---------------------------------|--|----------------------------|---|
| 141                             | High-symmetry tin(II) iodides as promising light absorbers for solar cells: A theoretical prediction. <i>Computational Materials Science</i> , <b>2019</b> , 156, 246-251  | 3.2                        | 1   |
| 140                             | DFT-derived atomic multipoles in AMOEBA force field for calculating intermolecular interactions of azabenzenes dimers. <i>Computational and Theoretical Chemistry</i> , <b>2018</b> , 1132, 35-41  | 2                          | 3   |
| 139                             | N-Modified NiO Surface for Superior Alkaline Hydrogen Evolution. <i>ChemSusChem</i> , <b>2018</b> , 11, 1020-1024  | 8.3                        | 9   |
| 138                             | Notable hydrogen production on LaxCa1\( \text{LCoO3} \) perovskites via two-step thermochemical water splitting. <i>Journal of Materials Science</i> , <b>2018</b> , 53, 6796-6806   | 4.3                        | 15  |
| 137                             | Enhanced Thermochemical H2 Production on Ca-Doped Lanthanum Manganite Perovskites Through Optimizing the Dopant Level and Re-oxidation Temperature. <i>Acta Metallurgica Sinica (English Letters)</i> , <b>2018</b> , 31, 431-439  | 2.5                        | 6   |
| 136                             | Enhanced gas sensing properties to NO2 of SnO2/rGO nanocomposites synthesized by microwave-assisted gas-liquid interfacial method. <i>Ceramics International</i> , <b>2018</b> , 44, 4900-4907   | 5.1                        | 26  |
| 135                             | Direct monitoring of spin transitions in a dinuclear triple-stranded helicate iron(ii) complex through X-ray photoelectron spectroscopy. <i>Dalton Transactions</i> , <b>2018</b> , 47, 2543-2548  | 4.3                        | 18  |
| 134                             | Electrolyte Effect on Electrocatalytic Hydrogen Evolution Performance of One-Dimensional CobaltDithiolene MetalDrganic Frameworks: A Theoretical Perspective. <i>ACS Applied Energy Materials</i> , <b>2018</b> , 1, 1688-1694   | 6.1                        | 14  |
|                                 |  |                            |   |
| 133                             | Iron Vacancies Induced Bifunctionality in Ultrathin Feroxyhyte Nanosheets for Overall Water Splitting. <i>Advanced Materials</i> , <b>2018</b> , 30, e1803144  | 24                         | 160   |
| 133                             |  | 24                         | 160<br>44   |
|                                 | Splitting. Advanced Materials, 2018, 30, e1803144  Sandwich-Like Reduced Graphene Oxide/Carbon Black/Amorphous Cobalt Borate Nanocomposites as Bifunctional Cathode Electrocatalyst in Rechargeable Zinc-Air Batteries. Advanced Energy  |                            | 44  |
| 132                             | Splitting. Advanced Materials, 2018, 30, e1803144  Sandwich-Like Reduced Graphene Oxide/Carbon Black/Amorphous Cobalt Borate Nanocomposites as Bifunctional Cathode Electrocatalyst in Rechargeable Zinc-Air Batteries. Advanced Energy Materials, 2018, 8, 1801495  Preparation of 1TNPhase ReSSe (x = 0-1) Nanodots for Highly Efficient Electrocatalytic Hydrogen   | 21.8                       | 44  |
| 132                             | Splitting. Advanced Materials, 2018, 30, e1803144  Sandwich-Like Reduced Graphene Oxide/Carbon Black/Amorphous Cobalt Borate Nanocomposites as Bifunctional Cathode Electrocatalyst in Rechargeable Zinc-Air Batteries. Advanced Energy Materials, 2018, 8, 1801495  Preparation of 1TNPhase ReSSe (x = 0-1) Nanodots for Highly Efficient Electrocatalytic Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2018, 140, 8563-8568  Bimetallic Carbide as a Stable Hydrogen Evolution Catalyst in Harsh Acidic Water. ACS Energy  | 21.8                       | 77  |
| 132<br>131<br>130               | Splitting. Advanced Materials, 2018, 30, e1803144  Sandwich-Like Reduced Graphene Oxide/Carbon Black/Amorphous Cobalt Borate Nanocomposites as Bifunctional Cathode Electrocatalyst in Rechargeable Zinc-Air Batteries. Advanced Energy Materials, 2018, 8, 1801495  Preparation of 1TNPhase ReSSe (x = 0-1) Nanodots for Highly Efficient Electrocatalytic Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2018, 140, 8563-8568  Bimetallic Carbide as a Stable Hydrogen Evolution Catalyst in Harsh Acidic Water. ACS Energy Letters, 2018, 3, 78-84  Remarkably enhanced water splitting activity of nickel foam due to simple immersion in a ferric   | 21.8<br>16.4<br>20.1       | <ul><li>44</li><li>77</li><li>35</li></ul>                      |
| 132<br>131<br>130               | Splitting. Advanced Materials, 2018, 30, e1803144  Sandwich-Like Reduced Graphene Oxide/Carbon Black/Amorphous Cobalt Borate Nanocomposites as Bifunctional Cathode Electrocatalyst in Rechargeable Zinc-Air Batteries. Advanced Energy Materials, 2018, 8, 1801495  Preparation of 1TNPhase ReSSe (x = 0-1) Nanodots for Highly Efficient Electrocatalytic Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2018, 140, 8563-8568  Bimetallic Carbide as a Stable Hydrogen Evolution Catalyst in Harsh Acidic Water. ACS Energy Letters, 2018, 3, 78-84  Remarkably enhanced water splitting activity of nickel foam due to simple immersion in a ferric nitrate solution. Nano Research, 2018, 11, 3959-3971  | 21.8<br>16.4<br>20.1       | <ul><li>44</li><li>77</li><li>35</li><li>45</li></ul>           |
| 132<br>131<br>130<br>129<br>128 | Sandwich-Like Reduced Graphene Oxide/Carbon Black/Amorphous Cobalt Borate Nanocomposites as Bifunctional Cathode Electrocatalyst in Rechargeable Zinc-Air Batteries. Advanced Energy Materials, 2018, 8, 1801495  Preparation of 1TNPhase ReSSe ( x = 0-1) Nanodots for Highly Efficient Electrocatalytic Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2018, 140, 8563-8568  Bimetallic Carbide as a Stable Hydrogen Evolution Catalyst in Harsh Acidic Water. ACS Energy Letters, 2018, 3, 78-84  Remarkably enhanced water splitting activity of nickel foam due to simple immersion in a ferric nitrate solution. Nano Research, 2018, 11, 3959-3971  ElTriketone-Monoterpene Hybrids from the Flowers of the Australian Tree Corymbia intermedia. Journal of Natural Products, 2018, 81, 2455-2461  Carbon nanodot aqueous binding phase-based diffusive gradients in thin films device for measurement of dissolved copper and lead species in the aquatic environment. Analyst, The, 2018, | 21.8<br>16.4<br>20.1<br>10 | <ul><li>44</li><li>77</li><li>35</li><li>45</li><li>2</li></ul> |

| 124 | Ultrathin Nitrogen-Doped Holey Carbon@Graphene Bifunctional Electrocatalyst for Oxygen Reduction and Evolution Reactions in Alkaline and Acidic Media. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 16511-16515 | 16.4 | 190 |
|-----|---|------|-----|
| 123 | Revealing the Role of Electrocatalyst Crystal Structure on Oxygen Evolution Reaction with Nickel as an Example. <i>Small</i> , <b>2018</b> , 14, e1802895   | 11   | 13  |
| 122 | Feroxyhyte Nanosheets: Iron Vacancies Induced Bifunctionality in Ultrathin Feroxyhyte Nanosheets for Overall Water Splitting (Adv. Mater. 36/2018). <i>Advanced Materials</i> , <b>2018</b> , 30, 1870272                               | 24   | 13  |
| 121 | Cobalt Covalent Doping in MoS to Induce Bifunctionality of Overall Water Splitting. <i>Advanced Materials</i> , <b>2018</b> , 30, e1801450  | 24   | 273 |
| 120 | Ultrathin Transition Metal Dichalcogenide/3d Metal Hydroxide Hybridized Nanosheets to Enhance Hydrogen Evolution Activity. <i>Advanced Materials</i> , <b>2018</b> , 30, e1801171   | 24   | 134 |
| 119 | Enhanced Thermochemical Water Splitting through Formation of Oxygen Vacancy in La Sr BO (B=Cr, Mn, Fe, Co, and Ni) Perovskites. <i>ChemPlusChem</i> , <b>2018</b> , 83, 924-928   | 2.8  | 10  |
| 118 | Carbon Nanotubes in TiO Nanofiber Photoelectrodes for High-Performance Perovskite Solar Cells. <i>Advanced Science</i> , <b>2017</b> , 4, 1600504   | 13.6 | 65  |
| 117 | Fabrication and assembly of two-dimensional TiO2/WO3IH2O heterostructures with type II band alignment for enhanced photocatalytic performance. <i>Applied Surface Science</i> , <b>2017</b> , 403, 564-571                              | 6.7  | 23  |
| 116 | Water-soluble inorganic photocatalyst for overall water splitting. <i>Applied Catalysis B: Environmental</i> , <b>2017</b> , 209, 247-252   | 21.8 | 13  |
| 115 | Electrospun TiO2BiO2 fibres with hierarchical pores from phase separation. <i>CrystEngComm</i> , <b>2017</b> , 19, 2673-2680  | 3.3  | 17  |
| 114 | Triphasic 2D Materials by Vertically Stacking Laterally Heterostructured 2H-/1T?-MoS2 on Graphene for Enhanced Photoresponse. <i>Advanced Electronic Materials</i> , <b>2017</b> , 3, 1700024   | 6.4  | 25  |
| 113 | Evaluation of electronic polarization energy in oligoacene molecular crystals using the solvated supermolecular approach. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 14453-14461                                    | 3.6  | 6   |
| 112 | Carbon-encapsulated heazlewoodite nanoparticles as highly efficient and durable electrocatalysts for oxygen evolution reactions. <i>Nano Research</i> , <b>2017</b> , 10, 3522-3533   | 10   | 23  |
| 111 | Ca2+ and Ga3+ doped LaMnO3 perovskite as a highly efficient and stable catalyst for two-step thermochemical water splitting. <i>Sustainable Energy and Fuels</i> , <b>2017</b> , 1, 1013-1017   | 5.8  | 23  |
| 110 | Assessment of DFT functionals for calculating intermolecular interaction of nitrogen-containing heterocyclic complexes. <i>Theoretical Chemistry Accounts</i> , <b>2017</b> , 136, 1  | 1.9  | 2   |
| 109 | One-pot, two-step synthesis and photophysical properties of 2-(5-phenylindol-3-yl)benzimidazole derivatives. <i>RSC Advances</i> , <b>2017</b> , 7, 49374-49385   | 3.7  | 8   |
| 108 | La1-Ca Mn1-Al O3 perovskites as efficient catalysts for two-step thermochemical water splitting in conjunction with exceptional hydrogen yields. <i>Chinese Journal of Catalysis</i> , <b>2017</b> , 38, 1079-1086                      | 11.3 | 16  |
| 107 | Brlisted base site engineering of graphitic carbon nitride for enhanced photocatalytic activity.  Journal of Materials Chemistry A, <b>2017</b> , 5, 19227-19236  | 13   | 24  |

# (2016-2017)

| 106 | Pimentelamines A-C, Indole Alkaloids Isolated from the Leaves of the Australian Tree Flindersia pimenteliana. <i>Journal of Natural Products</i> , <b>2017</b> , 80, 3211-3217   | 4.9            | 20   |
|-----|--|----------------|------|
| 105 | Ultrathin metal <b>ö</b> rganic framework nanosheets for electrocatalytic oxygen evolution. <i>Nature Energy</i> , <b>2016</b> , 1,  | 62.3           | 1444 |
| 104 | Functionalization of perovskite thin films with moisture-tolerant molecules. <i>Nature Energy</i> , <b>2016</b> , 1,   | 62.3           | 369  |
| 103 | Multi-shelled metal oxides prepared via an anion-adsorption mechanism for lithium-ion batteries. <i>Nature Energy</i> , <b>2016</b> , 1,   | 62.3           | 304  |
| 102 | One-step solid phase synthesis of a highly efficient and robust cobalt pentlandite electrocatalyst for the oxygen evolution reaction. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 18314-18321               | 13             | 80   |
| 101 | Reparameterization of 12-6 Lennard-Jones potentials based on quantum mechanism results for novel tetrahedral N4 (Td) explosives. <i>Theoretical Chemistry Accounts</i> , <b>2016</b> , 135, 1                              | 1.9            | 3    |
| 100 | Molecular engineering of Ni-/Co-porphyrin multilayers on reduced graphene oxide sheets as bifunctional catalysts for oxygen evolution and oxygen reduction reactions. <i>Chemical Science</i> , <b>2016</b> , 7, 5640-5646 | 9.4            | 108  |
| 99  | The surface sulfur doping induced enhanced performance of cobalt catalysts in oxygen evolution reactions. <i>Chemical Communications</i> , <b>2016</b> , 52, 9450-3  | 5.8            | 34   |
| 98  | In-silico design of a new energetic material 1-Amino-5-nitrotetrazole with high energy and density. Computational Materials Science, 2016, 112, 67-74  | 3.2            | 11   |
| 97  | A general precursor strategy for one-dimensional titania with surface nanoprotrusion and tunable structural hierarchy. <i>CrystEngComm</i> , <b>2016</b> , 18, 1321-1328   | 3.3            | 6    |
| 96  | COInduced Phase Engineering: Protocol for Enhanced Photoelectrocatalytic Performance of 2D MoSINanosheets. <i>ACS Nano</i> , <b>2016</b> , 10, 2903-9  | 16.7           | 187  |
| 95  | A bioscaffolding strategy for hierarchical zeolites with a nanotube-trimodal network. <i>Chemical Science</i> , <b>2016</b> , 7, 1582-1587   | 9.4            | 12   |
| 94  | Highly Ordered Single Crystalline Nanowire Array Assembled Three-Dimensional Nb3O7(OH) and Nb2O5 Superstructures for Energy Storage and Conversion Applications. <i>ACS Nano</i> , <b>2016</b> , 10, 507-14                | 16.7           | 65   |
| 93  | Strongly Coupled CoCr2 O4 /Carbon Nanosheets as High Performance Electrocatalysts for Oxygen Evolution Reaction. <i>Small</i> , <b>2016</b> , 12, 2866-71  | 11             | 76   |
| 92  | Self-template fabrication of one-dimensional hollow and solid porous titania by chemically induced self-transformation. <i>CrystEngComm</i> , <b>2016</b> , 18, 5572-5579  | 3.3            | 2    |
| 91  | Phase-dependent enhancement for CO2 photocatalytic reduction over CeO2/TiO2 catalysts. <i>Catalysis Science and Technology</i> , <b>2016</b> , 6, 7967-7975  | 5.5            | 51   |
| 90  | Revisiting the calcination-induced multi-layer hollowing of electrospun solid fibers. <i>CrystEngComm</i> , <b>2016</b> , 18, 8637-8644  | 3.3            | 3    |
| 89  | Metal-organic frameworks as selectivity regulators for hydrogenation reactions. <i>Nature</i> , <b>2016</b> , 539, 76-8  | B <b>@</b> 0.4 | 925  |

| 88 | An in situ vapour phase hydrothermal surface doping approach for fabrication of high performance Co3O4 electrocatalysts with an exceptionally high S-doped active surface. <i>Chemical Communications</i> , <b>2015</b> , 51, 5695-7              | 5.8              | 41  |
|----|---|------------------|-----|
| 87 | Nitrogen-Doped Carbon Nanodots@Nanospheres as An Efficient Electrocatalyst for Oxygen Reduction Reaction. <i>Electrochimica Acta</i> , <b>2015</b> , 165, 7-13  | 6.7              | 32  |
| 86 | Rutile {111} Faceted TiO2 Film with High Ability for Selective Adsorption of Aldehyde. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 17680-17686  | 3.8              | 6   |
| 85 | Titania Tube-in-Tube Scaffolds with Multilength-Scale Structural Hierarchy and Structure-Enhanced Functional Performance. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 17552-17560   | 3.8              | 11  |
| 84 | A fluorescent quenching performance enhancing principle for carbon nanodot-sensitized aqueous solar cells. <i>Nano Energy</i> , <b>2015</b> , 13, 124-130   | 17.1             | 29  |
| 83 | A New Graphdiyne Nanosheet/Pt Nanoparticle-Based Counter Electrode Material with Enhanced Catalytic Activity for Dye-Sensitized Solar Cells. <i>Advanced Energy Materials</i> , <b>2015</b> , 5, 1500296  | 21.8             | 149 |
| 82 | A photochromic naphthopyran dye activated by the intramolecular hydrogen bond and its photodynamics in the ormosil matrix coating. <i>Journal of Sol-Gel Science and Technology</i> , <b>2015</b> , 73, 293-2                                     | 9 <del>8</del> 3 | 10  |
| 81 | Density Functional Studies of Stoichiometric Surfaces of Orthorhombic Hybrid Perovskite CH3NH3PbI3. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 1136-1145   | 3.8              | 64  |
| 80 | ZnxCd1\( \text{IdS}\) bacterial cellulose bionanocomposite foams with hierarchical architecture and enhanced visible-light photocatalytic hydrogen production activity. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 1709-1716      | 13               | 33  |
| 79 | Self-supported bimodal-pore structured nitrogen-doped carbon fiber aerogel as electrocatalyst for oxygen reduction reaction. <i>Electrochemistry Communications</i> , <b>2015</b> , 51, 6-10  | 5.1              | 44  |
| 78 | Biotemplated synthesis of hierarchically nanostructured TiO2 using cellulose and its applications in photocatalysis. <i>RSC Advances</i> , <b>2015</b> , 5, 1673-1679   | 3.7              | 15  |
| 77 | Fabrication of Two-Dimensional Lateral Heterostructures of WS2/WO3?H2O Through Selective Oxidation of Monolayer WS2. <i>Angewandte Chemie</i> , <b>2015</b> , 127, 15441-15445  | 3.6              | 32  |
| 76 | Fabrication of Two-Dimensional Lateral Heterostructures of WS2 /WO3 ?H2 O Through Selective Oxidation of Monolayer WS2. <i>Angewandte Chemie - International Edition</i> , <b>2015</b> , 54, 15226-30   | 16.4             | 93  |
| 75 | Nd1\(\textbf{Q}\)CaxFeO3 (x = 0, 0.3) Hollow Core\(\textbf{B}\)hell Microspheres for Ethanol Gas Sensing. <i>European Journal of Inorganic Chemistry</i> , <b>2015</b> , 2015, 5767-5772  | 2.3              | 3   |
| 74 | Electrodes: A New Graphdiyne Nanosheet/Pt Nanoparticle-Based Counter Electrode Material with Enhanced Catalytic Activity for Dye-Sensitized Solar Cells (Adv. Energy Mater. 12/2015). <i>Advanced Energy Materials</i> , <b>2015</b> , 5, n/a-n/a | 21.8             | 1   |
| 73 | Switching the photocatalytic activity of g-C3N4 by homogenous surface chemical modification with nitrogen residues and vacancies. <i>RSC Advances</i> , <b>2015</b> , 5, 21430-21433  | 3.7              | 18  |
| 72 | Adsorption and oxidation of oxalic acid on anatase TiO2 (001) surface: A density functional theory study. <i>Journal of Colloid and Interface Science</i> , <b>2015</b> , 454, 180-6  | 9.3              | 15  |
| 71 | The search for efficient electrocatalysts as counter electrode materials for dye-sensitized solar cells: mechanistic study, material screening and experimental validation. NPG Asia Materials, 2015, 2226-226                                    | 10.3             | 38  |

# (2014-2015)

| 70 | Improved conductivity of NdFeOIthrough partial substitution of Nd by Ca: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 29097-102   | 3.6  | 5   |
|----|--|------|-----|
| 69 | Carbon-armored Co9S8 nanoparticles as all-pH efficient and durable H2-evolving electrocatalysts. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2015</b> , 7, 980-8  | 9.5  | 273 |
| 68 | Photoelectrochemical determination of intrinsic kinetics of photoelectrocatalysis processes at {001} faceted anatase TiO2 photoanodes. <i>RSC Advances</i> , <b>2015</b> , 5, 12860-12865  | 3.7  | 16  |
| 67 | Density functional theory analysis of structural and electronic properties of orthorhombic perovskite CH3NH3PbI3. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 1424-9  | 3.6  | 284 |
| 66 | Stable isolated metal atoms as active sites for photocatalytic hydrogen evolution. <i>Chemistry - A European Journal</i> , <b>2014</b> , 20, 2138-44   | 4.8  | 132 |
| 65 | Formation Mechanism of Freestanding CH3NH3PbI3 Functional Crystals: In Situ Transformation vs Dissolution@rystallization. <i>Chemistry of Materials</i> , <b>2014</b> , 26, 6705-6710  | 9.6  | 130 |
| 64 | TiO2BiO2 composite fibers with tunable interconnected porous hierarchy fabricated by single-spinneret electrospinning toward enhanced photocatalytic activity. <i>Journal of Materials Chemistry A</i> , <b>2014</b> , 2, 12442  | 13   | 37  |
| 63 | A {0001} faceted single crystal NiS nanosheet electrocatalyst for dye-sensitised solar cells: sulfur-vacancy induced electrocatalytic activity. <i>Chemical Communications</i> , <b>2014</b> , 50, 5569-71   | 5.8  | 54  |
| 62 | Directly hydrothermal growth of ultrathin MoS2 nanostructured films as high performance counter electrodes for dye-sensitised solar cells. <i>RSC Advances</i> , <b>2014</b> , 4, 21277  | 3.7  | 70  |
| 61 | Reply to the <b>N</b> omment on "Density functional theory analysis of structural and electronic properties of orthorhombic perovskite CH3NH3PbI3"Nby J. Even et al., Phys. Chem. Chem. Phys., 2014, 10.1039/C3CP55006K. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 8699-700 | 3.6  | 2   |
| 60 | Zinc oxide aerogel-like materials with an intriguing interwoven hollow-sphere morphology for selective ethanol sensing. <i>RSC Advances</i> , <b>2014</b> , 4, 21815-21818   | 3.7  | 2   |
| 59 | Hydrothermal transformation of dried grass into graphitic carbon-based high performance electrocatalyst for oxygen reduction reaction. <i>Small</i> , <b>2014</b> , 10, 3371-8   | 11   | 122 |
| 58 | A self-sponsored doping approach for controllable synthesis of S and N co-doped trimodal-porous structured graphitic carbon electrocatalysts. <i>Energy and Environmental Science</i> , <b>2014</b> , 7, 3720-3726   | 35.4 | 180 |
| 57 | Determination of Iodide via Direct Fluorescence Quenching at Nitrogen-Doped Carbon Quantum Dot Fluorophores. <i>Environmental Science and Technology Letters</i> , <b>2014</b> , 1, 87-91  | 11   | 65  |
| 56 | Geometric structure of rutile titanium dioxide (111) surfaces. <i>Physical Review B</i> , <b>2014</b> , 90,  | 3.3  | 17  |
| 55 | The size and valence state effect of Pt on photocatalytic H2 evolution over platinized TiO2 photocatalyst. <i>International Journal of Hydrogen Energy</i> , <b>2014</b> , 39, 1237-1242   | 6.7  | 60  |
| 54 | Vapor-phase hydrothermal synthesis of rutile TiO[hanostructured film with exposed pyramid-shaped (111) surface and superiorly photoelectrocatalytic performance. <i>Journal of Colloid and Interface Science</i> , <b>2014</b> , 429, 53-61  | 9.3  | 21  |
| 53 | Removal of nitric oxide by the highly reactive anatase TiO2 (001) surface: a density functional theory study. <i>Journal of Colloid and Interface Science</i> , <b>2014</b> , 430, 18-23   | 9.3  | 20  |

| 52 | Effects of global orbital cutoff value and numerical basis set size on accuracies of theoretical atomization energies. <i>Theoretical Chemistry Accounts</i> , <b>2014</b> , 133, 1                                    | 1.9 | 18 |
|----|--|-----|----|
| 51 | Bottom-Up Enhancement of g-C3N4Photocatalytic H2Evolution Utilising Disordering Intermolecular Interactions of Precursor. <i>International Journal of Photoenergy</i> , <b>2014</b> , 2014, 1-8                        | 2.1 | 7  |
| 50 | Stable Isolated Metal Atoms as Active Sites for Photocatalytic Hydrogen Evolution. <i>Chemistry - A European Journal</i> , <b>2014</b> , 20, 2088-2088   | 4.8 | 2  |
| 49 | Preparation of a fast photochromic ormosil matrix coating for smart windows. <i>Journal of Materials Science</i> , <b>2013</b> , 48, 5862-5870   | 4.3 | 21 |
| 48 | Theoretical understanding and prediction of lithiated sodium hexatitanates. <i>ACS Applied Materials &amp; Amp; Interfaces</i> , <b>2013</b> , 5, 1108-12  | 9.5 | 9  |
| 47 | Determination of Sudan dyes in environmental water by magnetic mesoporous microsphere-based solid phase extraction ultra fast liquid chromatography. <i>Analytical Methods</i> , <b>2013</b> , 5, 1399                 | 3.2 | 24 |
| 46 | A highly crystalline Nb3O7F nanostructured photoelectrode: fabrication and photosensitisation. <i>Journal of Materials Chemistry A</i> , <b>2013</b> , 1, 6563   | 13  | 28 |
| 45 | Nature of visible-light responsive fluorinated titanium dioxides. <i>Journal of Materials Chemistry A</i> , <b>2013</b> , 1, 12948   | 13  | 24 |
| 44 | Rutile TiO2 films with 100% exposed pyramid-shaped (111) surface: photoelectron transport properties under UV and visible light irradiation. <i>Journal of Materials Chemistry A</i> , <b>2013</b> , 1, 2646           | 13  | 35 |
| 43 | Vapor-phase hydrothermal growth of novel segmentally configured nanotubular crystal structure. <i>Small</i> , <b>2013</b> , 9, 3043-50   | 11  | 8  |
| 42 | Edges of FeO/Pt(111) Interface: A First-Principle Theoretical Study. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 1672-1676   | 3.8 | 8  |
| 41 | Engineering the band gap of bare titanium dioxide materials for visible-light activity: a theoretical prediction. <i>RSC Advances</i> , <b>2013</b> , 3, 8777  | 3.7 | 29 |
| 40 | Directly hydrothermal growth of single crystal Nb3O7(OH) nanorod film for high performance dye-sensitized solar cells. <i>Advanced Materials</i> , <b>2012</b> , 24, 1598-603  | 24  | 74 |
| 39 | Improved UV resistance in wood through the hydrothermal growth of highly ordered ZnO nanorod arrays. <i>Journal of Materials Science</i> , <b>2012</b> , 47, 4457-4462   | 4.3 | 29 |
| 38 | Low temperature solvothermal synthesis of anatase TiO2 single crystals with wholly {100} and {001} faceted surfaces. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 23906                                   |     | 82 |
| 37 | Structure, reactivity, photoactivity and stability of Ti-O based materials: a theoretical comparison. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 2333-8  | 3.6 | 40 |
| 36 | Vertically aligned nanorod-like rutile TiO2 single crystal nanowire bundles with superior electron transport and photoelectrocatalytic properties. <i>Journal of Materials Chemistry</i> , <b>2012</b> , 22, 2465-2472 |     | 79 |
| 35 | Vapor-phase hydrothermal transformation of HTiOF3 intermediates into {001} faceted anatase single-crystalline nanosheets. <i>Small</i> , <b>2012</b> , 8, 3664-73  | 11  | 51 |

#### (2005-2012)

| 34 | Visible light active pure rutile TiO2 photoanodes with 100% exposed pyramid-shaped (111) surfaces. <i>Nano Research</i> , <b>2012</b> , 5, 762-769   | 10   | 46  |
|----|--|------|-----|
| 33 | Anatase TiOlærystal facet growth: mechanistic role of hydrofluoric acid and photoelectrocatalytic activity. <i>ACS Applied Materials &amp; Description</i> (2011), 3, 2472-8   | 9.5  | 95  |
| 32 | Chain-branching control of the atomic structure of alkanethiol-based gold-sulfur interfaces. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 14856-9  | 16.4 | 27  |
| 31 | A selective etching phenomenon on {001} faceted anatase titanium dioxide single crystal surfaces by hydrofluoric acid. <i>Chemical Communications</i> , <b>2011</b> , 47, 2829-31  | 5.8  | 117 |
| 30 | Facile fabrication of anatase TiO2 microspheres on solid substrates and surface crystal facet transformation from {001} to {101}. <i>Chemistry - A European Journal</i> , <b>2011</b> , 17, 5949-57                                  | 4.8  | 67  |
| 29 | A facile vapor-phase hydrothermal method for direct growth of titanate nanotubes on a titanium substrate via a distinctive nanosheet roll-up mechanism. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 19032-5 | 16.4 | 90  |
| 28 | Gold Mining by Alkanethiol Radicals: Vacancies and Pits in the Self-Assembled Monolayers of 1-Propanethiol and 1-Butanethiol on Au(111). <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 10630-10639                     | 3.8  | 32  |
| 27 | Origin of reactivity diversity of lattice oxygen in titanates. <i>Chemical Physics Letters</i> , <b>2011</b> , 511, 82-86  | 2.5  | 11  |
| 26 | Chemical analysis of the superatom model for sulfur-stabilized gold nanoparticles. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 8378-84  | 16.4 | 80  |
| 25 | Scanning Tunneling Microscopic Observation of Adatom-Mediated Motifs on GoldII hiol Self-Assembled Monolayers at High Coverage. <i>Journal of Physical Chemistry C</i> , <b>2009</b> , 113, 19601-19608                              | 3.8  | 26  |
| 24 | Understanding the Chemisorption of 2-Methyl-2-propanethiol on Au(111). <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 10878-10885   | 3.8  | 16  |
| 23 | Formation of gold-methanethiyl self-assembled monolayers. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 14532-3   | 16.4 | 39  |
| 22 | Successful a priori modeling of CO adsorption on Pt(111) using periodic hybrid density functional theory. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 10402-7   | 16.4 | 67  |
| 21 | The ManganiteWater Interface. <i>Journal of Physical Chemistry C</i> , <b>2007</b> , 111, 10427-10437  | 3.8  | 12  |
| 20 | Simulation of the Au(111)[22B) surface reconstruction. <i>Physical Review B</i> , <b>2007</b> , 75,  | 3.3  | 71  |
| 19 | Prediction of tetraoxygen formation on rutile TiO2(110). <i>Journal of the American Chemical Society</i> , <b>2006</b> , 128, 14000-1  | 16.4 | 44  |
| 18 | Nucleation and growth of 1B metal clusters on rutile TiO2(1 1 0): Atomic level understanding from first principles studies. <i>Catalysis Today</i> , <b>2005</b> , 105, 78-84  | 5.3  | 22  |
| 17 | P-assisted growth of molecular wires on Si(001)-2¶. Applied Physics Letters, 2005, 86, 023108  | 3.4  | 3   |

| 16 | Origin of nonlocal interactions in adsorption of polar molecules on Si(001)-2 x 1. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 164706  | 3.9  | 25 |
|----|--|------|----|
| 15 | Dynamics of oxygen species on reduced TiO2(110) rutile. <i>Physical Review B</i> , <b>2004</b> , 70,   | 3.3  | 57 |
| 14 | A comparative theoretical study of Au, Ag and Cu adsorption on TiO2 (110) rutile surfaces. <i>Korean Journal of Chemical Engineering</i> , <b>2004</b> , 21, 537-547   | 2.8  | 17 |
| 13 | Two-dimensional arrangement of CH3NH2 adsorption on Si(0 0 1)-2 🗓 . <i>Chemical Physics Letters</i> , <b>2004</b> , 385, 144-148   | 2.5  | 8  |
| 12 | Effects of Subsurface Boron and Phosphorus on Surface Reactivity of Si(001): Water and Ammonia Adsorption. <i>Journal of Physical Chemistry B</i> , <b>2004</b> , 108, 16147-16153                               | 3.4  | 3  |
| 11 | Function of subsurface boron on Si(0 0 1)-2 🗓: water adsorption. <i>Surface Science</i> , <b>2003</b> , 547, L882-L886   | 1.8  | 5  |
| 10 | Adsorption of Au atoms on stoichiometric and reduced TiO2(110) rutile surfaces: a first principles study. <i>Surface Science</i> , <b>2003</b> , 542, 72-80  | 1.8  | 83 |
| 9  | Theoretical Study of Atomic Oxygen Adsorption on the Chlorine-Modified Ag(111) Surface. <i>Journal of Physical Chemistry B</i> , <b>2003</b> , 107, 3813-3819  | 3.4  | 13 |
| 8  | Theoretical study about adsorption of atomic oxygen on unmodified and I-modified Ag(100) surface. <i>Journal of Chemical Physics</i> , <b>2003</b> , 118, 11210-11216  | 3.9  | 5  |
| 7  | O/Ag(100) Surface: A Density Functional Study with Slab Model. <i>Journal of Physical Chemistry B</i> , <b>2002</b> , 106, 3662-3667   | 3.4  | 26 |
| 6  | Interaction of halogen atom with Ag(1 1 0): ab initio pseudopotential density functional study. <i>Chemical Physics Letters</i> , <b>2001</b> , 334, 411-418   | 2.5  | 18 |
| 5  | The first-principle study of the iodine-modified silver surfaces. Surface Science, 2001, 487, 77-86  | 1.8  | 21 |
| 4  | Structural and electronic properties of silver surfaces: ab initio pseudopotential density functional study. <i>Surface Science</i> , <b>2001</b> , 490, 125-132   | 1.8  | 41 |
| 3  | Ab initio pseudopotential study of dehydrogenation of methanol on oxygen modified Ag(110) surface. <i>Surface Science</i> , <b>2000</b> , 459, 213-222   | 1.8  | 15 |
| 2  | Ru(bpy)32+-sensitized {001} facets LiCoO2 nanosheets catalyzed CO2 reduction reaction with 100% carbonaceous products. <i>Nano Research</i> ,1   | 10   | 6  |
| 1  | High-Efficiency Electrosynthesis of Hydrogen Peroxide from Oxygen Reduction Enabled by a Tungsten Single Atom Catalyst with Unique Terdentate N 1 O 2 Coordination. <i>Advanced Functional Materials</i> 2110224 | 15.6 | 10 |