# Jin Yong Lee

List of Publications by Year
in descending order



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|---|---|---|---|
| 352 papers | 17,860 citations | 11639 70 h-index | 19169 118 g-index |
| 353 all docs | 353 docs citations | 353 times ranked | 18573 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Synergistic ultra-high activity of double B doped graphyne for electrocatalytic nitrogen reduction. Chemical Engineering Journal, 2022, 428, 131318. | 6.6 | 26 |
| 2 | Activating Î³-graphyne nanoribbons as bifunctional electrocatalysts toward oxygen reduction and hydrogen evolution reactions by edge termination and nitrogen doping. Chemical Engineering Journal, 2022, 430, 133126. | 6.6 | 17 |
| 3 | Flameâ€Assisted Synthesis of Oâ€Coordinated Singleâ€Atom Catalysts for Efficient Electrocatalytic Oxygen Reduction and Hydrogen Evolution Reaction. Small Methods, 2022, 6, e2101324. | 4.6 | 14 |
| 4 | C6N3: A novel 2D carbon nitride with sp-N as support for efficient hydrogen production. Journal of Colloid and Interface Science, 2022, 611, 472-479. | 5.0 | 2 |
| 5 | A Facile, Proteinâ€Derived Supramolecular Theranostic Strategy for Multimodalâ€Imagingâ€Guided Photodynamic and Photothermal Immunotherapy In Vivo. Advanced Materials, 2022, 34, e2109111. | 11.1 | 40 |
| 6 | Mechanistic Insights into the Polymorphic Associations and Cross-Seeding of AÎ² and hIAPP in the Presence of Histidine Tautomerism: An All-Atom Molecular Dynamic Study. International Journal of Molecular Sciences, 2022, 23, 1930. | 1.8 | 2 |
| 7 | Time-Resolved Optical Pump-Resonant X-ray Probe Spectroscopy of 4-Thiouracil: A Simulation Study. Journal of Chemical Theory and Computation, 2022, 18, 3075-3088. | 2.3 | 7 |
| 8 | Graphyne Nanotubes as Promising Sodium-Ion Battery Anodes. Catalysts, 2022, 12, 670. | 1.6 | 4 |
| 9 | Histidine tautomerism dependent conformational transitions driven aggregation of profilin-1: Implications in amyotrophic lateral sclerosis. International Journal of Biological Macromolecules, 2022, 214, 241-251. | 3.6 | 5 |
| 10 | Insights into amyotrophic lateral sclerosis linked Pro525Arg mutation in the fused in sarcoma protein through in silico analysis and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5963-5976. | 2.0 | 6 |
| 11 | An Ethacrynic Acidâ€Brominated BODIPY Photosensitizer (EAâ€BPS) Construct Enhances the Lethality of Reactive Oxygen Species in Hypoxic Tumorâ€Targeted Photodynamic Therapy. Angewandte Chemie - International Edition, 2021, 60, 3196-3204. | 7.2 | 68 |
| 12 | A microfluidic cathodic photoelectrochemical biosensor chip for the targeted detection of cytokeratin 19 fragments 21-1. Lab on A Chip, 2021, 21, 378-384. | 3.1 | 29 |
| 13 | NiSn Atomic Pair on an Integrated Electrode for Synergistic Electrocatalytic CO<sub>2</sub> Reduction. Angewandte Chemie - International Edition, 2021, 60, 7382-7388. | 7.2 | 137 |
| 14 | An Ethacrynic Acidâ€Brominated BODIPY Photosensitizer (EAâ€BPS) Construct Enhances the Lethality of Reactive Oxygen Species in Hypoxic Tumorâ€Targeted Photodynamic Therapy. Angewandte Chemie, 2021, 133, 3233-3241. | 1.6 | 6 |
| 15 | Harnessing Î±-<scp>l</scp>-fucosidase for in vivo cellular senescence imaging. Chemical Science, 2021, 12, 10054-10062. | 3.7 | 25 |
| 16 | Molecular mechanism of amyloidogenicity and neurotoxicity of a pro-aggregated tau mutant in the presence of histidine tautomerism via replica-exchange simulation. Physical Chemistry Chemical Physics, 2021, 23, 10475-10486. | 1.3 | 10 |
| 17 | Site-dependent photoinduced charge carrier dynamics in nitrogen/fluorine doped TiO2 nanoparticles. Journal of Materials Chemistry C, 2021, 9, 1992-2000. | 2.7 | 0 |
| 18 | Perpendicularly anchored ReSe2 nanoflakes on reduced graphene oxide support for highly efficient hydrogen evolution reactions. Chemical Engineering Journal, 2021, 405, 126728. | 6.6 | 29 |

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|---|---|---|---|
| 19 | NiSn Atomic Pair on an Integrated Electrode for Synergistic Electrocatalytic CO<sub>2</sub> Reduction. Angewandte Chemie, 2021, 133, 7458-7464. | 1.6 | 25 |
| 20 | Adsorption of [<scp>BF<sub>4</sub></scp>]<sup>â^'</sup> anionâ€based ionic liquids on phosphorene, arsenene, and antimonene: A density functional theory study. International Journal of Quantum Chemistry, 2021, 121, e26668. | 1.0 | 3 |
| 21 | Theoretical insights into the mechanism of oxygen evolution reaction (OER) on pristine BiVO<sub>4</sub> (001) and BiVO<sub>4</sub> (110) surfaces in acidic medium both in the gas and solution (water) phases. Nanotechnology, 2021, 32, 335401. | 1.3 | 3 |
| 22 | Ozone Decomposition on Defective Graphene: Insights from Modeling. Journal of Physical Chemistry C, 2021, 125, 10948-10954. | 1.5 | 4 |
| 23 | Histidine Tautomeric Effect on the Key Fragment R3 of Tau Protein from Atomistic Simulations. ACS Chemical Neuroscience, 2021, 12, 1983-1988. | 1.7 | 10 |
| 24 | Electronically coupled layered double hydroxide/<scp>MXene</scp> quantum dot metallic hybrids for highâ€performance flexible zincâ€“air batteries. InformaÄnÃ-MateriÃ¡ly, 2021, 3, 1134-1144. | 8.5 | 73 |
| 25 | Synergistic Molecular Engineering of Holeâ€Injecting Conducting Polymers Overcomes Luminescence Quenching in Perovskite Lightâ€Emitting Diodes. Advanced Optical Materials, 2021, 9, 2100646. | 3.6 | 14 |
| 26 | A simple general descriptor for rational design of graphyne-based bifunctional electrocatalysts toward hydrogen evolution and oxygen reduction reactions. Journal of Colloid and Interface Science, 2021, 592, 440-447. | 5.0 | 22 |
| 27 | Unveiling Trifunctional Active Sites of a Heteronanosheet Electrocatalyst for Integrated Cascade Battery/Electrolyzer Systems. ACS Energy Letters, 2021, 6, 2460-2468. | 8.8 | 42 |
| 28 | Histidine Tautomerism Driving Human Islet Amyloid Polypeptide Aggregation in the Early Stages of Diabetes Mellitus Progression: Insight at the Atomistic Level. Chemistry - an Asian Journal, 2021, 16, 2453-2462. | 1.7 | 6 |
| 29 | Mitochondria-targeted nanotheranostic: Harnessing single-laser-activated dual phototherapeutic processing for hypoxic tumor treatment. Matter, 2021, 4, 2508-2521. | 5.0 | 22 |
| 30 | Role of the English (H6R) Mutation on the Structural Properties of AÎ²40 and AÎ²42 Owing to the Histidine Tautomeric Effect. ACS Chemical Neuroscience, 2021, 12, 2705-2711. | 1.7 | 2 |
| 31 | Unraveling the Histidine Tautomerism Effect on the Initial Stages of Prion Misfolding: New Insights from a Computational Perspective. ACS Chemical Neuroscience, 2021, 12, 3203-3213. | 1.7 | 7 |
| 32 | Molecular insight into the early stage of amyloid-Î²(1-42) Homodimers aggregation influenced by histidine tautomerism. International Journal of Biological Macromolecules, 2021, 184, 887-897. | 3.6 | 8 |
| 33 | Supertetrahedraphene: A novel quasi 2D carbon allotrope with controllable thickness and electronic properties. Chemical Physics, 2021, 548, 111257. | 0.9 | 3 |
| 34 | Insight into the histidine tautomerism effect on heterodimers of AÎ²40. Bulletin of the Korean Chemical Society, 2021, 42, 1549-1554. | 1.0 | 3 |
| 35 | Hollow performances quenching label of Au NPs@CoSnO3 nanoboxes-based sandwich photoelectrochemical immunosensor for sensitive CYFRA 21-1 detection. Talanta, 2021, 233, 122552. | 2.9 | 9 |
| 36 | New design strategy for chemically-stable blue phosphorescent materials: improving the energy gap between the T<sub>1</sub> and <sup>3</sup>MC states. Physical Chemistry Chemical Physics, 2021, 23, 3543-3551. | 1.3 | 7 |

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|---|---|---|---|
| 37 | Acetylene coupler builds strong and tunable diradical organic molecular magnets. New Journal of Chemistry, 2021, 45, 9137-9142. | 1.4 | 0 |
| 38 | Porous CoSe<sub>2</sub>@N-doped carbon nanowires: an ultra-high stable and large-current-density oxygen evolution electrocatalyst. Chemical Communications, 2021, 57, 1774-1777. | 2.2 | 27 |
| 39 | Protein-Activatable Diarylethene Monomer as a Smart Trigger of Noninvasive Control Over Reversible Generation of Singlet Oxygen: A Facile, Switchable, Theranostic Strategy for Photodynamic-Immunotherapy. Journal of the American Chemical Society, 2021, 143, 2413-2422. | 6.6 | 72 |
| 40 | Theoretical Insights into Mutation and Histidine Tautomerism Effects on Tau Proteins. ACS Chemical Neuroscience, 2021, 12, 4361-4366. | 1.7 | 5 |
| 41 | Conical Intersection Passages of Molecules Probed by X-ray Diffraction and Stimulated Raman Spectroscopy. Journal of Physical Chemistry Letters, 2021, 12, 12300-12309. | 2.1 | 17 |
| 42 | The nano gold rush: Graphynes as atomic sieves for coinage and Pt-group transition metals. Applied Surface Science, 2020, 499, 143927. | 3.1 | 5 |
| 43 | Covalently decorated crown ethers on magnetic graphene oxides as bi-functional adsorbents with tailorable ion recognition properties for selective metal ion capture in water. Chemical Engineering Journal, 2020, 389, 123421. | 6.6 | 50 |
| 44 | Enhanced Catalytic Oxidation of CO on Sulfurâ€Doped Boron Nitride. ChemNanoMat, 2020, 6, 223-231. | 1.5 | 11 |
| 45 | Kinetically controlled Ag<sup>+</sup>-coordinated chiral supramolecular polymerization accompanying a helical inversion. Chemical Science, 2020, 11, 721-730. | 3.7 | 30 |
| 46 | The key role of acceptor moieties on the structural and the electronic properties of thermally activated delayed fluorescence emitters in excited states: A computational study. Organic Electronics, 2020, 78, 105595. | 1.4 | 10 |
| 47 | Monitoring aromatic ring-currents in Mg-porphyrin by time-resolved circular dichroism. Physical Chemistry Chemical Physics, 2020, 22, 26605-26613. | 1.3 | 6 |
| 48 | Asymmetric synthesis of Î³-chiral borylalkanes via sequential reduction/hydroboration using a single copper catalyst. Chemical Science, 2020, 11, 8961-8965. | 3.7 | 4 |
| 49 | N^N Pt(II) Bisacetylide Complexes with Oxoverdazyl Radical Ligands: Preparation, Photophysical Properties, and Magnetic Exchange Interaction between the Two Radical Ligands. Inorganic Chemistry, 2020, 59, 12471-12485. | 1.9 | 5 |
| 50 | Tautomeric Effect of Histidine on Î²-Sheet Formation of Amyloid Beta 1â€“40: 2D-IR Simulations. Biophysical Journal, 2020, 119, 831-842. | 0.2 | 9 |
| 51 | Intrinsic Origin of Tau Protein Aggregation: Effects of Histidine Tautomerism on Tau<sub>267â€“312</sub> Monomer. ACS Chemical Neuroscience, 2020, 11, 3814-3822. | 1.7 | 12 |
| 52 | Advancement of Platinum (Pt)-Free (Non-Pt Precious Metals) and/or Metal-Free (Non-Precious-Metals) Electrocatalysts in Energy Applications: A Review and Perspectives. Energy & Fuels, 2020, 34, 6634-6695. | 2.5 | 100 |
| 53 | Methylation Detection and DNA Sequencing Based on Adsorption of Nucleobases on Silicene Nanoribbon. Journal of Physical Chemistry C, 2020, 124, 10823-10831. | 1.5 | 12 |
| 54 | Impact of A2V Mutation and Histidine Tautomerism on AÎ²42 Monomer Structures from Atomistic Simulations. Journal of Chemical Information and Modeling, 2020, 60, 3587-3592. | 2.5 | 18 |

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| 55 | Î³-Graphyne nanotubes as defect-free catalysts of the oxygen reduction reaction: a DFT investigation. Physical Chemistry Chemical Physics, 2020, 22, 8633-8638. | 1.3 | 17 |
| 56 | GeC/GaN vdW Heterojunctions: A Promising Photocatalyst for Overall Water Splitting and Solar Energy Conversion. ACS Applied Materials & Interfaces, 2020, 12, 14289-14297. | 4.0 | 62 |
| 57 | H-Bonding on spin centres enhances spinâ€“spin coupling for organic diradicals. Journal of Materials Chemistry C, 2020, 8, 3402-3408. | 2.7 | 8 |
| 58 | Graphyne-anchored single Fe atoms as efficient CO oxidation catalysts as predicted by DFT calculations. Physical Chemistry Chemical Physics, 2020, 22, 6004-6009. | 1.3 | 10 |
| 59 | Anionic Redox Chemistry as a Clue for Understanding the Structural Behavior in Layered Cathode Materials. Small, 2020, 16, e1905875. | 5.2 | 21 |
| 60 | Catalytic nature of iron-nitrogen-graphene heterogeneous catalysts for oxygen evolution reaction and oxygen reduction reaction. Applied Surface Science, 2020, 514, 146073. | 3.1 | 15 |
| 61 | Synergy of sp-N and sp<sup>2</sup>-N codoping endows graphdiyne with comparable oxygen reduction reaction performance to Pt. Nanoscale, 2019, 11, 16599-16605. | 2.8 | 25 |
| 62 | Intrinsic Origin of Amyloid Aggregation: Collective Effects of the Mutation and Tautomerism of Histidine. ACS Chemical Neuroscience, 2019, 10, 4729-4734. | 1.7 | 18 |
| 63 | Signatures of Throughâ€Space Charge Transfer in Twoâ€Photon Absorption of Paracyclophane Derivatives. Bulletin of the Korean Chemical Society, 2019, 40, 1076-1086. | 1.0 | 2 |
| 64 | Structural and Binding Properties on AÎ² Mature Fibrils Due to the Histidine Tautomeric Effect. ACS Chemical Neuroscience, 2019, 10, 4612-4618. | 1.7 | 18 |
| 65 | Controllable oxygen-incorporated interlayer-expanded ReS<sub>2</sub> nanosheets deposited on hollow mesoporous carbon spheres for improved redox kinetics of Li-ion storage. Journal of Materials Chemistry A, 2019, 7, 22070-22078. | 5.2 | 10 |
| 66 | Design of efficient non-doped blue emitters: toward the improvement of charge transport. RSC Advances, 2019, 9, 27807-27816. | 1.7 | 3 |
| 67 | 3D PtAu nanoframe superstructure as a high-performance carbon-free electrocatalyst. Nanoscale, 2019, 11, 2840-2847. | 2.8 | 27 |
| 68 | Singular Nonmagnetic Semiconductor ScH<sub>3</sub> Molecular Nanowire: A New Type of Room-Temperature Spintronic Material. Journal of Physical Chemistry C, 2019, 123, 16994-17001. | 1.5 | 7 |
| 69 | Anchoring CuO Nanoparticles On C, Nâ€Codoped Gâ€C<sub>3</sub>N<sub>4</sub> Nanosheets from Melamineâ€Entrapped MOF Gel for Highâ€Efficiency Oxygen Evolution. ChemNanoMat, 2019, 5, 1170-1175. | 1.5 | 8 |
| 70 | Origin of structural stability of ScH3 molecular nanowires and their chemical-bonding behavior: Correlation effects of the Sc 3d electrons. Journal of Chemical Physics, 2019, 150, 184307. | 1.2 | 8 |
| 71 | Strong Influence of Oxygen Vacancy Location on Charge Carrier Losses in Reduced TiO<sub>2</sub> Nanoparticles. Journal of Physical Chemistry Letters, 2019, 10, 2676-2683. | 2.1 | 32 |
| 72 | Photocatalytic activity of TiO<sub>2</sub>nanoparticles: a theoretical aspect. Journal of Materials Chemistry A, 2019, 7, 13833-13859. | 5.2 | 153 |

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| 73 | High capacity conversion anodes in Li-ion batteries: A review. International Journal of Hydrogen Energy, 2019, 44, 10852-10905. | 3.8 | 88 |
| 74 | Electric Field Effect on Condensed-Phase Molecular Systems. VII. Vibrational Stark Sensitivity of Spatially Oriented Water Molecules in an Argon Matrix. Journal of Physical Chemistry C, 2019, 123, 9868-9874. | 1.5 | 12 |
| 75 | Supramolecular complexation of homocysteine and cysteine with cucurbit[7]uril. Supramolecular Chemistry, 2019, 31, 369-376. | 1.5 | 4 |
| 76 | Intrinsic origin of amyloid aggregation: Behavior of histidine (ÎµÎµÎµ) and (ÎÎÎ) tautomer homodimers of AÎ² (1â€“40). Biochimica Et Biophysica Acta - General Subjects, 2019, 1863, 795-801. | 1.1 | 27 |
| 77 | Electrocatalytic property of water oxidation reaction depends on charging state of intermediates on Ag-M (M = Fe, co, Ni, Cu) in alkaline media. International Journal of Hydrogen Energy, 2019, 44, 5863-5871. | 3.8 | 5 |
| 78 | Chiral Î³-graphyne nanotubes with almost equivalent bandgaps. Journal of Chemical Physics, 2019, 150, 054706. | 1.2 | 11 |
| 79 | Tautomerization Effect of Histidines on Oligomer Aggregation of Î²-Amyloid(1â€“40/42) during the Early Stage: Tautomerism Hypothesis for Misfolding Protein Aggregation. ACS Chemical Neuroscience, 2019, 10, 2602-2608. | 1.7 | 27 |
| 80 | Metal-organic framework-derived core-shell-structured nitrogen-doped CoCx/FeCo@C hybrid supported by reduced graphene oxide sheets as high performance bifunctional electrocatalysts for ORR and OER. Journal of Catalysis, 2019, 371, 185-195. | 3.1 | 78 |
| 81 | Monoamine oxidase-A targeting probe for prostate cancer imaging and inhibition of metastasis. Chemical Communications, 2019, 55, 13267-13270. | 2.2 | 25 |
| 82 | Bidirectional heterostructures consisting of graphene and lateral MoS<sub>2</sub>/WS<sub>2</sub> composites: a first-principles study. RSC Advances, 2019, 9, 34986-34994. | 1.7 | 4 |
| 83 | Reduced graphene Oxide/Poly(1,5 dihydroxynaphthalene)/TiO2 nanocomposite conducting polymer coated on gold as a supercapacitor electrode. Electrochimica Acta, 2019, 298, 726-734. | 2.6 | 29 |
| 84 | Phase Cycling RT-TDDFT Simulation Protocol for Nonlinear XUV and X-ray Molecular Spectroscopy. Journal of Physical Chemistry Letters, 2018, 9, 1072-1078. | 2.1 | 13 |
| 85 | Inhibition of corrosion of aluminum in alkaline solution by a novel azo-schiff base: Experiment and theory. Journal of Alloys and Compounds, 2018, 746, 185-193. | 2.8 | 47 |
| 86 | Size and Shape Effects on Charge Recombination Dynamics of TiO<sub>2</sub> Nanoclusters. Journal of Physical Chemistry C, 2018, 122, 5201-5208. | 1.5 | 39 |
| 87 | Bioinspired Synthesis of Chiral 3,4-Dihydropyranones via S-to-O Acyl-Transfer Reactions. Organic Letters, 2018, 20, 1584-1588. | 2.4 | 24 |
| 88 | Highly sensitive and selective electrochemical sensor for detection of vitamin B12 using an Au/PPy/FMNPs@TD-modified electrode. Sensors and Actuators B: Chemical, 2018, 261, 335-344. | 4.0 | 47 |
| 89 | Network-controlled unique reactivities of carbonyl groups in hollow and microporous organic polymer. Chemical Communications, 2018, 54, 5134-5137. | 2.2 | 16 |
| 90 | Polyaniline/aluminum and iron oxide nanocomposites supercapacitor electrodes with high specific capacitance and surface area. Journal of Electroanalytical Chemistry, 2018, 810, 100-108. | 1.9 | 62 |

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| 91 | Impact of Topology of Alkoxy Side Chain in Alkoxyphenylthiophene Subsituted Benzodithiophene Based 2D Conjugated Low Bandgap Polymers on Photophysical and Photovoltaic Properties. Macromolecular Research, 2018, 26, 500-505. | 1.0 | 9 |
| 92 | Î³-Al2O3 nanoparticle catalyst mediated polyaniline gold electrode biosensor for vitamin E. Catalysis Communications, 2018, 110, 59-63. | 1.6 | 20 |
| 93 | Attosecond X-ray Diffraction Triggered by Core or Valence Ionization of a Dipeptide. Journal of Chemical Theory and Computation, 2018, 14, 329-338. | 2.3 | 16 |
| 94 | Development of a theranostic prodrug for colon cancer therapy by combining ligand-targeted delivery and enzyme-stimulated activation. Biomaterials, 2018, 155, 145-151. | 5.7 | 85 |
| 95 | Electroic and optical properties of germanene/MoS2 heterobilayers: first principles study. Journal of Molecular Modeling, 2018, 24, 333. | 0.8 | 12 |
| 96 | Modeling realistic titania nanoparticles. Frontiers of Nanoscience, 2018, 12, 205-238. | 0.3 | 2 |
| 97 | Photocatalytic properties of intrinsically defective undoped bismuth vanadate (BiVO4) photocatalyst: A DFT study. Journal of Electroanalytical Chemistry, 2018, 828, 97-101. | 1.9 | 5 |
| 98 | Trigraphene and its Derivates: A Novel Carbon Allotrope. Bulletin of the Korean Chemical Society, 2018, 39, 1279-1282. | 1.0 | 7 |
| 99 | Theoretically Predicted New Multicyclic Compound by Stilbene Dimer. Bulletin of the Korean Chemical Society, 2018, 39, 1283-1286. | 1.0 | 1 |
| 100 | Oxygen reduction reaction (ORR) kinetics through different solvents of the non-aqueous electrolyte in Li-air (O2) batteries in both the gas and solution phases: A DFT study. Journal of Molecular Liquids, 2018, 271, 274-280. | 2.3 | 6 |
| 101 | Surface Functional Groups and Electrochemical Behavior in Dimethyl Sulfoxideâ€Đelaminated Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene. ChemSusChem, 2018, 11, 3719-3723. | 3.6 | 83 |
| 102 | Overcoming Drug Resistance by Targeting Cancer Bioenergetics with an Activatable Prodrug. CheM, 2018, 4, 2370-2383. | 5.8 | 85 |
| 103 | Sulfurâ€Doped CoO Nanoflakes with Loosely Packed Structure Realizing Enhanced Oxygen Evolution Reaction. Chemistry - A European Journal, 2018, 24, 17288-17292. | 1.7 | 39 |
| 104 | In Situ Water-Compatible Polymer Entrapment: A Strategy for Transferring Superhydrophobic Microporous Organic Polymers to Water. ACS Macro Letters, 2018, 7, 651-655. | 2.3 | 22 |
| 105 | Effective modulation of intramolecular ferromagnetic interaction of diradicals by functionalization of cross-conjugated coupler. Physical Chemistry Chemical Physics, 2018, 20, 20688-20694. | 1.3 | 6 |
| 106 | Effects of double-atom vacancies on the electronic properties of graphyne: a DFT investigation. Physical Chemistry Chemical Physics, 2018, 20, 22739-22743. | 1.3 | 8 |
| 107 | Electronic and Nuclear Contributions to Vibrational Stark Shifts of Hydroxyl Stretching Frequencies of Water Clusters. Journal of Physical Chemistry C, 2018, 122, 12970-12974. | 1.5 | 4 |
| 108 | Effect of Ru crystal phase on the catalytic activity of hydrolytic dehydrogenation of ammonia borane. Journal of Power Sources, 2018, 396, 148-154. | 4.0 | 34 |

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| 109 | Single-atom vacancy induced changes in electronic and magnetic properties of graphyne. Carbon, 2017, 116, 113-119. | 5.4 | 30 |
| 110 | Doping and vacancy effects of graphyne on SO2 adsorption. Journal of Colloid and Interface Science, 2017, 493, 123-129. | 5.0 | 30 |
| 111 | When Anatase Nanoparticles Become Bulklike: Properties of Realistic TiO<sub>2</sub> Nanoparticles in the 1â€“6 nm Size Range from All Electron Relativistic Density Functional Theory Based Calculations. Journal of Chemical Theory and Computation, 2017, 13, 1785-1793. | 2.3 | 87 |
| 112 | Visible-Light Driven Photocatalytic Degradation of Organic Dyes over Ordered Mesoporous Cd<sub>x</sub>Zn<sub>1â€“x</sub>S Materials. Journal of Physical Chemistry C, 2017, 121, 5137-5144. | 1.5 | 65 |
| 113 | Periodicity of band gaps of chiral Î±-graphyne nanotubes. Physical Chemistry Chemical Physics, 2017, 19, 7919-7922. | 1.3 | 11 |
| 114 | Systematic study of the effect of HSE functional internal parameters on the electronic structure and band gap of a representative set of metal oxides. Journal of Computational Chemistry, 2017, 38, 781-789. | 1.5 | 60 |
| 115 | Functionalization of Î³-graphyne by transition metal adatoms. Carbon, 2017, 120, 63-70. | 5.4 | 81 |
| 116 | Overcoming the Limits of Hypoxia in Photodynamic Therapy: A Carbonic Anhydrase IX-Targeted Approach. Journal of the American Chemical Society, 2017, 139, 7595-7602. | 6.6 | 261 |
| 117 | Cooperative Binding of Metal Cations to a Spiropyranâ€Conjugated Calix[4]arene. ChemistrySelect, 2017, 2, 3527-3533. | 0.7 | 4 |
| 118 | Atomic layer etching of graphene through controlled ion beam for graphene-based electronics. Scientific Reports, 2017, 7, 2462. | 1.6 | 31 |
| 119 | Atomic Layer Etching Mechanism of MoS<sub>2</sub> for Nanodevices. ACS Applied Materials & Interfaces, 2017, 9, 11967-11976. | 4.0 | 81 |
| 120 | Tautomeric Effect of Histidine on the Monomeric Structure of Amyloid Î²-Peptide(1â€“42). ACS Chemical Neuroscience, 2017, 8, 669-675. | 1.7 | 35 |
| 121 | Micro Galvanic Cell To Generate PtO and Extend the Triple-Phase Boundary during Self-Assembly of Pt/C and Nafion for Catalyst Layers of PEMFC. ACS Applied Materials & Interfaces, 2017, 9, 38165-38169. | 4.0 | 11 |
| 122 | Electric field effect on the magnetic properties of zigzag MoS2 nanoribbons with different edge passivation. Physical Chemistry Chemical Physics, 2017, 19, 30814-30821. | 1.3 | 4 |
| 123 | Calix[n]triazoles and Related Conformational Studies. Organic Letters, 2017, 19, 5509-5512. | 2.4 | 14 |
| 124 | Size-Dependent Level Alignment between Rutile and Anatase TiO<sub>2</sub> Nanoparticles: Implications for Photocatalysis. Journal of Physical Chemistry Letters, 2017, 8, 5593-5598. | 2.1 | 75 |
| 125 | Spectroelectrochemistry and electrosynthesis of polypyrrole supercapacitor electrodes based on gamma aluminum oxide and gamma iron (III) oxide nanocomposites. Electrochimica Acta, 2017, 251, 212-222. | 2.6 | 34 |
| 126 | Solution-processable highly efficient deep-red and orange organic light-emitting diodes based on multi-functional Ir(iii) complexes. Journal of Materials Chemistry C, 2017, 5, 10029-10038. | 2.7 | 20 |

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| 127 | PLK1-Targeted Fluorescent Tumor Imaging with High Signal-to-Background Ratio. ACS Sensors, 2017, 2, 1512-1516. | 4.0 | 20 |
| 128 | Copper-Catalyzed Enantioselective Hydroboration of Unactivated 1,1-Disubstituted Alkenes. Journal of the American Chemical Society, 2017, 139, 13660-13663. | 6.6 | 118 |
| 129 | Revealing the importance of nitrogen doping site in enhancing the oxygen reduction reaction on Î²-graphyne. Carbon, 2017, 123, 415-420. | 5.4 | 37 |
| 130 | Substrate-mediated single-atom isolation: dispersion of Ni and La on Î³-graphyne. Theoretical Chemistry Accounts, 2017, 136, 1. | 0.5 | 14 |
| 131 | Applying strong external electric field to thiopheneâ€based oligomers: A promising approach to upgrade semiconducting performance. Journal of Computational Chemistry, 2017, 38, 304-311. | 1.5 | 8 |
| 132 | Reduction potential tuning of first row transition metal MIII/MII (M = Cr, Mn, Fe, Co, Ni) hexadentate complexes for viable aqueous redox flow battery catholytes: A DFT study. Electrochimica Acta, 2017, 246, 156-164. | 2.6 | 8 |
| 133 | New benzodithiopheneâ€•and benzooxadiazole/benzothiadiazoleâ€based donorâ€“acceptor Ï€â€conjugated polymers for organic photovoltaics. Journal of Polymer Science Part A, 2016, 54, 2668-2679. | 2.5 | 7 |
| 134 | Effect of Size and Structure on the Ground-State and Excited-State Electronic Structure of TiO<sub>2</sub> Nanoparticles. Journal of Chemical Theory and Computation, 2016, 12, 3751-3763. | 2.3 | 53 |
| 135 | Solar Cells: Highly Efficient Organic Hole Transporting Materials for Perovskite and Organic Solar Cells with Long-Term Stability (Adv. Mater. 4/2016). Advanced Materials, 2016, 28, 685-685. | 11.1 | 0 |
| 136 | Performance of a modified hybrid functional in the simultaneous description of stoichiometric and reduced TiO<sub>2</sub>polymorphs. Physical Chemistry Chemical Physics, 2016, 18, 12357-12367. | 1.3 | 49 |
| 137 | Triazolium-promoted highly selective fluorescence â€œturn-onâ€•detection of fluoride ions. Dyes and Pigments, 2016, 132, 248-254. | 2.0 | 9 |
| 138 | Doping Effect on Edge-Terminated Ferromagnetic Graphene Nanoribbons. Journal of Physical Chemistry C, 2016, 120, 11237-11244. | 1.5 | 22 |
| 139 | Importance of doping site of B, N, and O in tuning electronic structure of graphynes. Carbon, 2016, 105, 156-162. | 5.4 | 46 |
| 140 | Copper-Catalyzed trans-Hydroboration of Terminal Aryl Alkynes: Stereodivergent Synthesis of Alkenylboron Compounds. Organic Letters, 2016, 18, 1390-1393. | 2.4 | 117 |
| 141 | Mitochondria-Targeted Reaction-Based Fluorescent Probe for Hydrogen Sulfide. Analytical Chemistry, 2016, 88, 5476-5481. | 3.2 | 213 |
| 142 | Single oxygen vacancies of (TiO<sub>2</sub>)<sub>35</sub>as a prototype reduced nanoparticle: implication for photocatalytic activity. Physical Chemistry Chemical Physics, 2016, 18, 23755-23762. | 1.3 | 35 |
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