## Srimanta Pakhira

List of Publications by Year in descending order

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| #  | Article   | IF  | CITATIONS |
|----|---|-----|-----------|
| 1  | Pyrene-based fluorescent Ru( <scp>ii</scp> )-arene complexes for significant biological applications:<br>catalytic potential, DNA/protein binding, two photon cell imaging and <i>in vitro</i> cytotoxicity.<br>Dalton Transactions, 2022, 51, 3937-3953.   | 1.6 | 14        |
| 2  | Hydrogen: A Future Chemical Fuel. Materials Horizons, 2022, , 1-30.   | 0.3 | 5         |
| 3  | Electrochemical Water Splitting: H2 Evolution Reaction. Materials Horizons, 2022, , 59-89.  | 0.3 | 2         |
| 4  | Efficient electrocatalytic H <sub>2</sub> evolution mediated by 2D Janus MoSSe transition metal dichalcogenide. Sustainable Energy and Fuels, 2022, 6, 1733-1752.   | 2.5 | 14        |
| 5  | H <sub>2</sub> physisorption on covalent organic framework linkers and metalated linkers: a strategy to enhance binding strength. Molecular Systems Design and Engineering, 2022, 7, 577-591.   | 1.7 | 7         |
| 6  | Large and Uniform Single Crystals of MoS <sub>2</sub> Monolayers for ppb-Level NO <sub>2</sub><br>Sensing. ACS Applied Nano Materials, 2022, 5, 9415-9426.  | 2.4 | 44        |
| 7  | Mechanism of electrochemical oxygen reduction reaction at two-dimensional Pt-doped<br>MoSe <sub>2</sub> material: an efficient electrocatalyst. Journal of Materials Chemistry C, 2021, 9,<br>11331-11342.  | 2.7 | 27        |
| 8  | Constructing a High-Performance Aqueous Rechargeable Zinc-Ion Battery Cathode with<br>Self-Assembled Mat-like Packing of Intertwined Ag(I) Pre-Inserted<br>V <sub>3</sub> O <sub>7</sub> ·H <sub>2</sub> O Microbelts with Reduced Graphene Oxide Core. ACS<br>Sustainable Chemistry and Engineering, 2021, 9, 3985-3995. | 3.2 | 40        |
| 9  | Selective anticancer activities of ruthenium(II)-tetrazole complexes and their mechanistic insights.<br>BioMetals, 2021, 34, 795-812.   | 1.8 | 6         |
| 10 | Rapidly Reversible Organic Crystalline Switch for Conversion of Heat into Mechanical Energy. Journal of the American Chemical Society, 2021, 143, 5951-5957.  | 6.6 | 29        |
| 11 | Recent advancements of two-dimensional transition metal dichalcogenides and their applications in electrocatalysis and energy storage. Emergent Materials, 2021, 4, 951-970.  | 3.2 | 24        |
| 12 | Generation of emissive nanosphere from micro-aggregates in anionic perylene diimide: Co-relation of self-assembly, emission, and electrical properties. Dyes and Pigments, 2021, 192, 109461.   | 2.0 | 4         |
| 13 | Tunability of the Electronic Properties of Covalent Organic Frameworks. ACS Applied Electronic Materials, 2021, 3, 720-732.   | 2.0 | 26        |
| 14 | Low temperature activation of inert hexagonal boron nitride for metal deposition and single atom catalysis. Materials Today, 2021, 51, 108-116.   | 8.3 | 16        |
| 15 | Unveiling the role of 2D monolayer Mn-doped MoS <sub>2</sub> material: toward an efficient<br>electrocatalyst for H <sub>2</sub> evolution reaction. Physical Chemistry Chemical Physics, 2021, 24,<br>265-280.   | 1.3 | 21        |
| 16 | Mechanistic Insight for Targeting Biomolecules by Ruthenium(II) NSAID Complexes. ACS Applied Bio<br>Materials, 2020, 3, 4600-4612.  | 2.3 | 11        |
| 17 | Catalyzing the Intercalation Storage Capacity of Aqueous Zinc-Ion Battery Constructed with Zn(II)<br>Preinserted Organo-Vanadyl Hybrid Cathode. ACS Applied Energy Materials, 2020, 3, 3425-3434.   | 2.5 | 27        |
| 18 | Quantum Nature in the Interaction of Molecular Hydrogen with Porous Materials: Implications for<br>Practical Hydrogen Storage. Journal of Physical Chemistry C, 2020, 124, 6454-6460.   | 1.5 | 12        |

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|----|--|------|-----------|
| 19 | Substituents Effects of Organic Linkers on Rotational Energy Barriers in Metalâ€Organic Frameworks.<br>ChemistrySelect, 2019, 4, 8584-8592.  | 0.7  | 14        |
| 20 | Energy framework approach to the supramolecular reactions: interplay of the secondary bonding<br>interaction in Ph <sub>2</sub> E <sub>2</sub> (E = Se, Te)/ <i>p</i> -I-C <sub>6</sub> F <sub>4</sub> -I<br>co-crystals. New Journal of Chemistry, 2019, 43, 7941-7949. | 1.4  | 22        |
| 21 | Intercalation of first row transition metals inside covalent-organic frameworks (COFs): a strategy to fine tune the electronic properties of porous crystalline materials. Physical Chemistry Chemical Physics, 2019, 21, 8785-8796.                                     | 1.3  | 28        |
| 22 | Raman and electrical transport properties of few-layered arsenic-doped black phosphorus. Nanoscale, 2019, 11, 18449-18463.   | 2.8  | 27        |
| 23 | Rotational dynamics of the organic bridging linkers in metal–organic frameworks and their substituent effects on the rotational energy barrier. RSC Advances, 2019, 9, 38137-38147.  | 1.7  | 24        |
| 24 | S-Doped MoP Nanoporous Layer Toward High-Efficiency Hydrogen Evolution in pH-Universal<br>Electrolyte. ACS Catalysis, 2019, 9, 651-659.  | 5.5  | 167       |
| 25 | Synthesis and Characterization of Tris-chelate Complexes for Understanding <i>f</i> -Orbital Bonding in Later Actinides. Journal of the American Chemical Society, 2019, 141, 2356-2366.   | 6.6  | 41        |
| 26 | Demystifying the Mechanism of Regio- and Isoselective Epoxide Polymerization Using the Vandenberg<br>Catalyst. Macromolecules, 2018, 51, 1777-1786.  | 2.2  | 26        |
| 27 | Apically Dominant Mechanism for Improving Catalytic Activities of Nâ€Doped Carbon Nanotube Arrays in<br>Rechargeable Zinc–Air Battery. Advanced Energy Materials, 2018, 8, 1800480.  | 10.2 | 153       |
| 28 | Modulating Electrocatalysis on Graphene Heterostructures: Physically Impermeable Yet<br>Electronically Transparent Electrodes. ACS Nano, 2018, 12, 2980-2990.  | 7.3  | 45        |
| 29 | Dirac cone in two dimensional bilayer graphene by intercalation with V, Nb, and Ta transition metals.<br>Journal of Chemical Physics, 2018, 148, 064707.   | 1.2  | 20        |
| 30 | Tuning the Dirac Cone of Bilayer and Bulk Structure Graphene by Intercalating First Row Transition<br>Metals Using First-Principles Calculations. Journal of Physical Chemistry C, 2018, 122, 4768-4782.   | 1.5  | 30        |
| 31 | Binderâ€Free ZnO Cathode synthesized via ALD by Direct Growth of Hierarchical ZnO Nanostructure on<br>Current Collector for Highâ€Performance Rechargeable Aluminiumâ€Ion Batteries. ChemistrySelect, 2018,<br>3, 12512-12523.   | 0.7  | 14        |
| 32 | Achieving Fast and Efficient K <sup>+</sup> Intercalation on Ultrathin Graphene Electrodes Modified<br>by a Li <sup>+</sup> Based Solid-Electrolyte Interphase. Journal of the American Chemical Society, 2018,<br>140, 13599-13603.                                     | 6.6  | 54        |
| 33 | Reaction mechanism of the selective reduction of CO <sub>2</sub> to CO by a tetraaza<br>[Co <sup>II</sup> N <sub>4</sub> H] <sup>2+</sup> complex in the presence of protons. Physical<br>Chemistry Chemical Physics, 2018, 20, 24058-24064.                             | 1.3  | 15        |
| 34 | Hybridization of Co <sub>3</sub> O <sub>4</sub> and α-MnO <sub>2</sub> Nanostructures for<br>High-Performance Nonenzymatic Glucose Sensing. ACS Sustainable Chemistry and Engineering, 2018, 6,<br>13248-13261.  | 3.2  | 54        |
| 35 | Low-temperature Synthesis of Heterostructures of Transition Metal Dichalcogenide Alloys<br>(W <sub><i>x</i></sub> Mo <sub>1–<i>x</i></sub> S <sub>2</sub> ) and Graphene with Superior Catalytic<br>Performance for Hydrogen Evolution. ACS Nano, 2017, 11, 5103-5112.   | 7.3  | 157       |
| 36 | Iron Intercalation in Covalent–Organic Frameworks: A Promising Approach for Semiconductors.<br>Journal of Physical Chemistry C, 2017, 121, 21160-21170.  | 1.5  | 46        |

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|----|---|-------------------|--------------|
| 37 | Quantum Monte Carlo Study of the Reactions of CH with Acrolein: Major and Minor Channels.<br>Journal of Physical Chemistry A, 2016, 120, 3602-3612.   | 1.1               | 21           |
| 38 | Interactions between metal cations with H2 in the M+- H2 complexes: Performance of DFT and DFT-D methods. Journal of Chemical Sciences, 2016, 128, 621-631.   | 0.7               | 16           |
| 39 | Diverse Rotational Flexibility of Substituted Dicarboxylate Ligands in Functional Porous<br>Coordination Polymers. Journal of Physical Chemistry C, 2015, 119, 28789-28799.   | 1.5               | 31           |
| 40 | Control of Diffusion and Conformation Behavior of Methyl Methacrylate Monomer by Phenylene Fin<br>in Porous Coordination Polymers. Journal of Physical Chemistry C, 2015, 119, 27291-27297.   | 1.5               | 10           |
| 41 | A Quantum Monte Carlo Study of the Reactions of CH with Acrolein. Journal of Physical Chemistry A, 2015, 119, 4214-4223.  | 1.1               | 28           |
| 42 | Theoretical study of efficiency of metal cations (Mg <sup>+</sup> , Ca <sup>+</sup> , and) Tj ETQq0 0 0 rgBT /Ov  | verlock 10<br>0.8 | Tf 50 542 Td |
| 43 | Association reaction between SiH3 and H2O2: a computational study of the reaction mechanism and kinetics. Theoretical Chemistry Accounts, 2013, 132, 1.   | 0.5               | 7            |
| 44 | Binding affinity of substituted ureidoâ€benzenesulfonamide ligands to the carbonic anhydrase<br>receptor: A theoretical study of enzyme inhibition. Journal of Computational Chemistry, 2013, 34,<br>1907-1916.                       | 1.5               | 5            |
| 45 | Performance of dispersion-corrected double hybrid density functional theory: A computational study of OCS-hydrocarbon van der Waals complexes. Journal of Chemical Physics, 2013, 138, 164319.  | 1.2               | 25           |
| 46 | Structure, stability, and dissociation of small ionic silicon oxide clusters [SiOn+(n = 3, 4)]: Insight from density functional and topological exploration. Journal of Chemical Physics, 2013, 139, 234303.                          | 1.2               | 7            |
| 47 | Dispersion corrected double high-hybrid and gradient-corrected density functional theory study of<br>light cation–dihydrogen (M+–H2, where MÂ=ÂLi, Na, B and Al) van der Waals complexes. Structural<br>Chemistry, 2013, 24, 549-558. | 1.0               | 16           |
| 48 | A Computational Study of Detoxification of Lewisite Warfare Agents by British Anti-lewisite: Catalytic<br>Effects of Water and Ammonia on Reaction Mechanism and Kinetics. Journal of Physical Chemistry A,                           | 1.1               | 19           |

| 48 | Effects of Water and Ammonia on Reaction Mechanism and Kinetics. Journal of Physical Chemistry A, 2013, 117, 3496-3506.  | 1.1 | 19 |
|----|--|-----|----|
| 49 | Can two T-shaped isomers of OCS–C2H2 van der Waals complex exist?. Chemical Physics Letters, 2012, 549, 6-11.  | 1.2 | 16 |
| 50 | Theoretical study of spectroscopy, interaction, and dissociation of linear and T-shaped isomers of RgClF (RgÂ=ÂHe, Ne, and Ar) van der Waals complexes. Structural Chemistry, 2012, 23, 681-692. | 1.0 | 8  |
| 51 | Coupled cluster study of structural properties of RgI and RgIâ^' (RgÂ=ÂHe, Ne, Ar) weakly bound<br>molecules. Structural Chemistry, 2011, 22, 893-900.   | 1.0 | 5  |
| 52 | Spectroscopy and dissociation of I2–Rg (RgÂ=ÂKr and Xe) van der Waals complexes. Theoretical<br>Chemistry Accounts, 2011, 130, 95-101.   | 0.5 | 14 |
| 53 | Spectroscopic properties of I2–Rg (Rg=He, Ne, Ar) van der Waals complexes. Chemical Physics Letters, 2011, 505, 81-86.   | 1.2 | 15 |