Mahesh Kumar Ravva

List of Publications by Year
in descending order

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65 papers	2,119 citations	257357 24 h-index	233338 45 g-index
67 all docs	67 docs citations	67 times ranked	3591 citing authors

#	Article	IF	Citations
1	A novel class of rigid-rod perylene diimides and isoindigo semiconducting polymers. Polymer Chemistry, 2022, 13, 536-544.	1.9	5
2	Simultaneous interaction of graphene nanoflakes with cations and anions: A cooperativity study. Computational and Theoretical Chemistry, 2022, 1209, 113601.	1.1	4
3	Theoretical insights into molecular design of hot-exciton based thermally activated delayed fluorescence molecules. Materials Advances, 2022, 3, 4954-4963.	2.6	12
4	Engineering colloidally stable, highly fluorescent and nontoxic Cu nanoclusters via reaction parameter optimization. RSC Advances, 2022, 12, 17585-17595.	1.7	5
5	Stereoselective Addition of Alkynes to Ketenimines: Copper/Amine Catalyzed Sulfonyl Azideâ€“Alkyne Cycloaddition Reactions for the Synthesis of (Z)-1,3-Enynes. Organic Letters, 2022, 24, 4310-4315.	2.4	0
6	Effect of Alkoxy Side-Chains on Conjugated Polymer/Non-fullerene Acceptor Interfaces in Organic Solar Cells. Journal of Electronic Materials, 2021, 50, 1713-1719.	1.0	0
7	Insights into the Ground-State Charge Transfer in Conjugated Polymer Donorâ€“Acceptor Complexes. Journal of Electronic Materials, 2021, 50, 1621-1628.	1.0	1
8	Synthesis of ortho-arylated and alkenylated benzamides by palladium-catalyzed denitrogenative cross-coupling reactions of 1,2,3-benzotriazin-4(3H)-ones with organoboronic acids. New Journal of Chemistry, 2021, 45, 17190-17195.	1.4	10
9	Fused ambipolar aza-isoindigos with NIR absorption. Organic Chemistry Frontiers, 2021, 8, 1170-1176.	2.3	4
10	Harnessing the Extracellular Electron Transfer Capability of Geobacter sulfurreducens for Ambient Synthesis of Stable Bifunctional Singleâ€Atom Electrocatalyst for Water Splitting. Advanced Functional Materials, 2021, 31, 2010916.	7.8	11
11	Electrochemical Energy Storage: Harnessing the Extracellular Electron Transfer Capability of Geobacter sulfurreducens for Ambient Synthesis of Stable Bifunctional Singleâ€Atom Electrocatalyst for Water Splitting (Adv. Funct. Mater. 22/2021). Advanced Functional Materials, 2021, 31, 2170161.	7.8	0
12	Theoretical Study on Understanding the Effects of Core Structure and Energy Level Tuning on Efficiency of Nonfullerene Acceptors in Organic Solar Cells. Advanced Theory and Simulations, 2021, 4, 2100019.	1.3	5
13	Novel and asymmetric S,N-heterocyclics with fused six-membered rings for organic field effect transistor applications. Journal of Materials Chemistry C, 2020, 8, 17083-17089.	2.7	3
14	Effect of halogenated substituent on the properties of aza-octacenes. Organic Electronics, 2020, 85, 105895.	1.4	6
15	A Novel Mitigation Mechanism for Photoâ€Induced Trapping in an Anthradithiophene Derivative Using Additives. Advanced Electronic Materials, 2020, 6, 2000250.	2.6	5
16	Benchmark studies on protonated benzene (BZH+) and water (Wn, nâ€‰=â€‰1â€“6) clusters: a comparison of hybrid DFT with MP2/CBS and CCSD(T)/CBS methods. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	4
17	Metal-free polymerization: synthesis and properties of fused benzo[1,2-b:4,5-bâ€²]bis[b]benzothiophene (BBBT) polymers. Polymer Chemistry, 2020, 11, 3695-3700.	1.9	6
18	Blue LED Mediated Intramolecular Câ€“H Functionalization and Cyclopropanation of Tryptamines: Synthesis of Azepino[4, 5-b]indoles and Natural Product Inspired Polycyclic Indoles. Organic Letters, 2020, 22, 4537-4541.	2.4	20

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19	Twisted Eigen Can Induce Proton Transfer at a Hydrophobicâ€“Hydrophilic Interface. Journal of Physical Chemistry A, 2020, 124, 3364-3373.	1.1	5
20	Harnessing Autoxidation of Aldehydes: In Situ Iodoarene Catalyzed Synthesis of Substituted 1,3,4-Oxadiazole, in the Presence of Molecular Oxygen. Organic Letters, 2019, 21, 6562-6565.	2.4	20
21	The synthesis and properties of a new class of Ï€-expanded diketopyrrolopyrrole analogs and conjugated polymers. Organic Chemistry Frontiers, 2019, 6, 2974-2980.	2.3	13
22	Fused Pyrazineâ€•and Carbazoleâ€Containing Azaacenes: Synthesis and Properties. ChemPlusChem, 2019, 84, 1257-1262.	1.3	5
23	Effect of conjugation length on the properties of fused perylene diimides with variable isoindigos. Journal of Materials Chemistry C, 2019, 7, 12263-12269.	2.7	12
24	Interactions of thiol and alkoxy radical with coinage metal nanoclusters. Applied Surface Science, 2019, 487, 1409-1419.	3.1	2
25	Directing-Group-Assisted Manganese-Catalyzed Cyclopropanation of Indoles. Organic Letters, 2019, 21, 2025-2028.	2.4	32
26	Cobalt-Catalyzed, Hydroxyl-Assisted Câ€“H Bond Functionalization: Access to Diversely Substituted Polycyclic Pyrans. Journal of Organic Chemistry, 2019, 84, 1176-1184.	1.7	27
27	Charge and Triplet Exciton Generation in Neat PC₇₀BM Films and Hybrid CuSCN:PC₇₀BM Solar Cells. Advanced Energy Materials, 2019, 9, 1802476.	10.2	20
28	Fused electron deficient semiconducting polymers for air stable electron transport. Nature Communications, 2018, 9, 416.	5.8	133
29	Bulk Heterojunction Solar Cells: Impact of Minor Structural Modifications to the Polymer Backbone on the Polymerâ€“Fullerene Mixing and Packing and on the Fullereneâ€“Fullerene Connecting Network. Advanced Functional Materials, 2018, 28, 1705868.	7.8	30
30	Impact of solution temperature-dependent aggregation on the solid-state packing and electronic properties of polymers for organic photovoltaics. Journal of Materials Chemistry C, 2018, 6, 13162-13170.	2.7	25
31	Synthesis and properties of isoindigo and benzo[1,2-b:4,5-bâ€²]bis[b]benzothiophene oligomers. Chemical Communications, 2018, 54, 11152-11155.	2.2	9
32	Co-operativity in non-covalent interactions in ternary complexes: a comprehensive electronic structure theory based investigation. Journal of Molecular Modeling, 2018, 24, 258.	0.8	4
33	Copper-Catalyzed Ring-Expansion Cascade of Azirines with Alkynes: Synthesis of Multisubstituted Pyridines at Room Temperature. Organic Letters, 2018, 20, 3241-3244.	2.4	29
34	High operational and environmental stability of high-mobility conjugated polymer field-effect transistors through the use of molecular additives. Nature Materials, 2017, 16, 356-362.	13.3	345
35	Charge-Transfer Dynamics in the Lowest Excited State of a Pentaceneâ€“Fullerene Complex: Implications for Organic Solar Cells. Journal of Physical Chemistry Letters, 2017, 8, 5171-5176.	2.1	28
36	Structural variations to a donor polymer with low energy losses. Journal of Materials Chemistry A, 2017, 5, 18618-18626.	5.2	12

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37	Computational Methodologies for Developing Structureâ€“Morphologyâ€“Performance Relationships in Organic Solar Cells: A Protocol Review. Chemistry of Materials, 2017, 29, 346-354.	3.2	61
38	Molecular Understanding of Fullerene â€“ Electron Donor Interactions in Organic Solar Cells. Advanced Energy Materials, 2017, 7, 1601370.	10.2	66
39	Noncovalent Interactions in Organic Electronic Materials. , 2017, , 277-302.		10
40	Impact of the Nature of the Sideâ€Chains on the Polymerâ€Fullerene Packing in the Mixed Regions of Bulk Heterojunction Solar Cells. Advanced Functional Materials, 2016, 26, 5913-5921.	7.8	45
41	Ionization Energies, Electron Affinities, and Polarization Energies of Organic Molecular Crystals: Quantitative Estimations from a Polarizable Continuum Model (PCM)-Tuned Range-Separated Density Functional Approach. Journal of Chemical Theory and Computation, 2016, 12, 2906-2916.	2.3	124
42	Benchmarking Density Functional Theory Approaches for the Description of Symmetry Breaking in Long Polymethine Dyes. Journal of Physical Chemistry C, 2016, 120, 9975-9984.	1.5	25
43	Effect of Molecular Packing and Charge Delocalization on the Nonradiative Recombination of Chargeâ€Transfer States in Organic Solar Cells. Advanced Energy Materials, 2016, 6, 1601325.	10.2	103
44	Effect of Substituents on the Electronic Structure and Degradation Process in Carbazole Derivatives for Blue OLED Host Materials. Chemistry of Materials, 2016, 28, 5791-5798.	3.2	83
45	Impact of Fluorine Substituents on Ï€â€Conjugated Polymer Mainâ€Chain Conformations, Packing, and Electronic Couplings. Advanced Materials, 2016, 28, 8197-8205.	11.1	78
46	Nature of the Binding Interactions between Conjugated Polymer Chains and Fullerenes in Bulk Heterojunction Organic Solar Cells. Chemistry of Materials, 2016, 28, 8181-8189.	3.2	34
47	Limits for Recombination in a Low Energy Loss Organic Heterojunction. ACS Nano, 2016, 10, 10736-10744.	7.3	79
48	Controllable molecular aggregation and fluorescence properties of 1,3,4-oxadiazole derivatives. Journal of Materials Chemistry C, 2015, 3, 11681-11688.	2.7	21
49	Supramolecular Functionalization and Concomitant Enhancement in Properties of Au₂₅ Clusters. ACS Nano, 2014, 8, 139-152.	7.3	94
50	Effects of functionalization of carbon nanotubes on their dispersion in an ethylene glycolâ€“water binary mixture â€“ a molecular dynamics and ONIOM investigation. Physical Chemistry Chemical Physics, 2014, 16, 24509-24518.	1.3	8
51	Theoretical study on molecular packing and electronic structure of bi-1,3,4-oxadiazole derivatives. RSC Advances, 2014, 4, 51942-51949.	1.7	7
52	Structure and Stability of (NG)_nCN₃Be₃⁺ Clusters and Comparison with (NG)BeY^{0/+}. ChemPhysChem, 2013, 14, 2511-2517.	1.0	41
53	Interaction of ethylene glycolâ€“water clusters with aromatic surfaces. RSC Advances, 2013, 3, 7798.	1.7	5
54	Studies on the Encapsulation of F^{â€“} in Single Walled Nanotubes of Different Chiralities Using Density Functional Theory Calculations and Carâ€“Parrinello Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2012, 116, 5519-5528.	1.1	13

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55	Improving the hydrogen storage capacity of metal organic framework by chemical functionalization. International Journal of Hydrogen Energy, 2012, 37, 16070-16077.	3.8	30
56	On the Perturbation of the H-Bonding Interaction in Ethylene Glycol Clusters upon Hydration. Journal of Physical Chemistry A, 2012, 116, 4239-4247.	1.1	83
57	Interaction of Carbon Nanotube with Ethylene Glycolâ€“Water Binary Mixture: A Molecular Dynamics and Density Functional Theory Investigation. Journal of Physical Chemistry C, 2012, 116, 4365-4373.	1.5	32
58	Density functional studies on the hydrogen storage capacity of boranes and alanes based cages. International Journal of Hydrogen Energy, 2012, 37, 9730-9741.	3.8	17
59	Density Functional Theory Studies on Ice Nanotubes. Journal of Physical Chemistry A, 2011, 115, 12841-12851.	1.1	9
60	Quantum Mechanical Studies on Interaction of Carbohydrate with Nanomaterials. Journal of Biomedical Nanotechnology, 2011, 7, 188-190.	0.5	2
61	Interaction of H2 with fragments of MOF-5 and its implications for the design and development of new MOFs: A computational study. International Journal of Hydrogen Energy, 2011, 36, 10737-10747.	3.8	18
62	Expedient synthesis of coumarin-coupled triazoles via â€˜click chemistryâ€™ leading to the formation of coumarinâ€“triazoleâ€“sugar hybrids. Carbohydrate Research, 2010, 345, 2297-2304.	1.1	26
63	Carbohydrate-Aromatic Interactions: The Role of Curvature on XHÂ·Â·Â·Ï€ Interactions. Journal of Physical Chemistry A, 2010, 114, 4313-4324.	1.1	35
64	Studies on the Structure and Stability of Cyclic Peptide Based Nanotubes Using Oligomeric Approach: A Computational Chemistry Investigation. Journal of Physical Chemistry B, 2010, 114, 16574-16583.	1.2	29
65	Ab Initio and DFT Studies on Methanolâ^'Water Clusters. Journal of Physical Chemistry A, 2010, 114, 2250-2258.	1.1	89