

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	High operational and environmental stability of high-mobility conjugated polymer field-effect transistors through the use of molecular additives. <i>Nature Materials</i> , 2017, 16, 356-362.	13.3	345
2	Fused electron deficient semiconducting polymers for air stable electron transport. <i>Nature Communications</i> , 2018, 9, 416.	5.8	133
3	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. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2906-2916.	2.3	124
4	Effect of Molecular Packing and Charge Delocalization on the Nonradiative Recombination of Charge Transfer States in Organic Solar Cells. <i>Advanced Energy Materials</i> , 2016, 6, 1601325.	10.2	103
5	Supramolecular Functionalization and Concomitant Enhancement in Properties of Au ₂₅ Clusters. <i>ACS Nano</i> , 2014, 8, 139-152.	7.3	94
6	Ab Initio and DFT Studies on Methanol-Water Clusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2250-2258.	1.1	89
7	On the Perturbation of the H-Bonding Interaction in Ethylene Glycol Clusters upon Hydration. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4239-4247.	1.1	83
8	Effect of Substituents on the Electronic Structure and Degradation Process in Carbazole Derivatives for Blue OLED Host Materials. <i>Chemistry of Materials</i> , 2016, 28, 5791-5798.	3.2	83
9	Limits for Recombination in a Low Energy Loss Organic Heterojunction. <i>ACS Nano</i> , 2016, 10, 10736-10744.	7.3	79
10	Impact of Fluorine Substituents on Conjugated Polymer Main Chain Conformations, Packing, and Electronic Couplings. <i>Advanced Materials</i> , 2016, 28, 8197-8205.	11.1	78
11	Molecular Understanding of Fullerene Electron Donor Interactions in Organic Solar Cells. <i>Advanced Energy Materials</i> , 2017, 7, 1601370.	10.2	66
12	Computational Methodologies for Developing Structure-Morphology-Performance Relationships in Organic Solar Cells: A Protocol Review. <i>Chemistry of Materials</i> , 2017, 29, 346-354.	3.2	61
13	Impact of the Nature of the Side Chains on the Polymer-Fullerene Packing in the Mixed Regions of Bulk Heterojunction Solar Cells. <i>Advanced Functional Materials</i> , 2016, 26, 5913-5921.	7.8	45
14	Structure and Stability of (NG) _n CN ₃ Be ₃ ⁺ Clusters and Comparison with (NG)BeY ⁺ . <i>ChemPhysChem</i> , 2013, 14, 2511-2517.	1.0	41
15	Carbohydrate-Aromatic Interactions: The Role of Curvature on XH...I Interactions. <i>Journal of Physical Chemistry A</i> , 2010, 114, 4313-4324.	1.1	35
16	Nature of the Binding Interactions between Conjugated Polymer Chains and Fullerenes in Bulk Heterojunction Organic Solar Cells. <i>Chemistry of Materials</i> , 2016, 28, 8181-8189.	3.2	34
17	Interaction of Carbon Nanotube with Ethylene Glycol-Water Binary Mixture: A Molecular Dynamics and Density Functional Theory Investigation. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4365-4373.	1.5	32
18	Directing-Group-Assisted Manganese-Catalyzed Cyclopropanation of Indoles. <i>Organic Letters</i> , 2019, 21, 2025-2028.	2.4	32

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19	Improving the hydrogen storage capacity of metal organic framework by chemical functionalization. International Journal of Hydrogen Energy, 2012, 37, 16070-16077.	3.8	30
20	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
21	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
22	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
23	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
24	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
25	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
26	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
27	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
28	Controllable molecular aggregation and fluorescence properties of 1,3,4-oxadiazole derivatives. Journal of Materials Chemistry C, 2015, 3, 11681-11688.	2.7	21
29	Harnessing Autoxidation of Aldehydes: <i>In Situ</i> Iodoarene Catalyzed Synthesis of Substituted 1,3,4-Oxadiazole, in the Presence of Molecular Oxygen. Organic Letters, 2019, 21, 6562-6565.	2.4	20
30	Charge and Triplet Exciton Generation in Neat PC ₇₀ BM Films and Hybrid CuSCN:PC ₇₀ BM Solar Cells. Advanced Energy Materials, 2019, 9, 1802476.	10.2	20
31	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
32	Interaction of H ₂ 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
33	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
34	Studies on the Encapsulation of F ⁺ 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
35	The synthesis and properties of Î€-expanded diketopyrrolopyrrole analogs and conjugated polymers. Organic Chemistry Frontiers, 2019, 6, 2974-2980.	2.3	13
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	Effect of conjugation length on the properties of fused perylene diimides with variable isoindigos. <i>Journal of Materials Chemistry C</i> , 2019, 7, 12263-12269.	2.7	12
38	Theoretical insights into molecular design of hot-exciton based thermally activated delayed fluorescence molecules. <i>Materials Advances</i> , 2022, 3, 4954-4963.	2.6	12
39	Harnessing the Extracellular Electron Transfer Capability of <i>Geobacter sulfurreducens</i> for Ambient Synthesis of Stable Bifunctional Single-Atom Electrocatalyst for Water Splitting. <i>Advanced Functional Materials</i> , 2021, 31, 2010916.	7.8	11
40	Noncovalent Interactions in Organic Electronic Materials. , 2017, , 277-302.		10
41	Synthesis of <i>ortho</i> -arylated and alkenylated benzamides by palladium-catalyzed denitrogenative cross-coupling reactions of 1,2,3-benzotriazin-4(3 <i>H</i>)-ones with organoboronic acids. <i>New Journal of Chemistry</i> , 2021, 45, 17190-17195.	1.4	10
42	Density Functional Theory Studies on Ice Nanotubes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12841-12851.	1.1	9
43	Synthesis and properties of isoindigo and benzo[1,2- <i>b</i> :4,5- <i>b'</i>]-bis[<i>b</i>]benzothiophene oligomers. <i>Chemical Communications</i> , 2018, 54, 11152-11155.	2.2	9
44	Effects of functionalization of carbon nanotubes on their dispersion in an ethylene glycol-water binary mixture – a molecular dynamics and ONIOM investigation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24509-24518.	1.3	8
45	Theoretical study on molecular packing and electronic structure of bi-1,3,4-oxadiazole derivatives. <i>RSC Advances</i> , 2014, 4, 51942-51949.	1.7	7
46	Effect of halogenated substituent on the properties of aza-octacenes. <i>Organic Electronics</i> , 2020, 85, 105895.	1.4	6
47	Metal-free polymerization: synthesis and properties of fused benzo[1,2- <i>b</i> :4,5- <i>b'</i>]-bis[<i>b</i>]benzothiophene (BBBT) polymers. <i>Polymer Chemistry</i> , 2020, 11, 3695-3700.	1.9	6
48	Interaction of ethylene glycol-water clusters with aromatic surfaces. <i>RSC Advances</i> , 2013, 3, 7798.	1.7	5
49	Fused Pyrazine- and Carbazole-Containing Azaacenes: Synthesis and Properties. <i>ChemPlusChem</i> , 2019, 84, 1257-1262.	1.3	5
50	A Novel Mitigation Mechanism for Photo-Induced Trapping in an Anthradithiophene Derivative Using Additives. <i>Advanced Electronic Materials</i> , 2020, 6, 2000250.	2.6	5
51	Twisted Eigen Can Induce Proton Transfer at a Hydrophobic-Hydrophilic Interface. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3364-3373.	1.1	5
52	Theoretical Study on Understanding the Effects of Core Structure and Energy Level Tuning on Efficiency of Nonfullerene Acceptors in Organic Solar Cells. <i>Advanced Theory and Simulations</i> , 2021, 4, 2100019.	1.3	5
53	A novel class of rigid-rod perylene diimides and isoindigo semiconducting polymers. <i>Polymer Chemistry</i> , 2022, 13, 536-544.	1.9	5
54	Engineering colloidally stable, highly fluorescent and nontoxic Cu nanoclusters <i>via</i> reaction parameter optimization. <i>RSC Advances</i> , 2022, 12, 17585-17595.	1.7	5

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55	Co-operativity in non-covalent interactions in ternary complexes: a comprehensive electronic structure theory based investigation. <i>Journal of Molecular Modeling</i> , 2018, 24, 258.	0.8	4
56	Benchmark studies on protonated benzene (BZH+) and water (W _n , n=1-6) clusters: a comparison of hybrid DFT with MP2/CBS and CCSD(T)/CBS methods. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	0.5	4
57	Fused ambipolar aza-isoindigos with NIR absorption. <i>Organic Chemistry Frontiers</i> , 2021, 8, 1170-1176.	2.3	4
58	Simultaneous interaction of graphene nanoflakes with cations and anions: A cooperativity study. <i>Computational and Theoretical Chemistry</i> , 2022, 1209, 113601.	1.1	4
59	Novel and asymmetric S,N-heterocyclics with fused six-membered rings for organic field effect transistor applications. <i>Journal of Materials Chemistry C</i> , 2020, 8, 17083-17089.	2.7	3
60	Quantum Mechanical Studies on Interaction of Carbohydrate with Nanomaterials. <i>Journal of Biomedical Nanotechnology</i> , 2011, 7, 188-190.	0.5	2
61	Interactions of thiol and alkoxy radical with coinage metal nanoclusters. <i>Applied Surface Science</i> , 2019, 487, 1409-1419.	3.1	2
62	Insights into the Ground-State Charge Transfer in Conjugated Polymer Donor-Acceptor Complexes. <i>Journal of Electronic Materials</i> , 2021, 50, 1621-1628.	1.0	1
63	Effect of Alkoxy Side-Chains on Conjugated Polymer/Non-fullerene Acceptor Interfaces in Organic Solar Cells. <i>Journal of Electronic Materials</i> , 2021, 50, 1713-1719.	1.0	0
64	Electrochemical Energy Storage: Harnessing the Extracellular Electron Transfer Capability of <i>Geobacter sulfurreducens</i> for Ambient Synthesis of Stable Bifunctional Single-Atom Electrocatalyst for Water Splitting (<i>Adv. Funct. Mater.</i> 22/2021). <i>Advanced Functional Materials</i> , 2021, 31, 2170161.	7.8	0
65	Stereoselective Addition of Alkynes to Ketenimines: Copper/Amine Catalyzed Sulfonyl Azide-Alkyne Cycloaddition Reactions for the Synthesis of <i>Z</i> -1,3-Enynes. <i>Organic Letters</i> , 2022, 24, 4310-4315.	2.4	0