

W M Chamil Sameera

List of Publications by Year in descending order

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70
papers

2,915
citations

257357

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175177

52
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80
all docs

80
docs citations

80
times ranked

3966
citing authors

#	ARTICLE	IF	CITATIONS
1	Modelling the Radical Chemistry on Ice Surfaces: An Integrated Quantum Chemical and Experimental Approach. <i>Frontiers in Astronomy and Space Sciences</i> , 2022, 9, .	1.1	4
2	Transition metal catalyzed cross-coupling and nitrogen reduction reactions: Lessons from computational studies. <i>Advances in Organometallic Chemistry</i> , 2022, , 35-78.	0.5	1
3	CO Binding onto Heterometals of [Mo ₃ S ₄ M] (M = Fe, Co, Ni) Cubes. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 1190-1195.	2.0	2
4	Nitrogen reduction by the Fe sites of synthetic [Mo ₃ S ₄ Fe] cubes. <i>Nature</i> , 2022, 607, 86-90.	13.7	55
5	Synthesis, characterization and biological evaluation of dipicolylamine sulfonamide derivatized platinum complexes as potential anticancer agents. <i>RSC Advances</i> , 2021, 11, 17658-17668.	1.7	5
6	Palladium-Catalyzed Regioselective and Stereospecific Ring-Opening Suzuki-Miyaura Arylative Cross-Coupling of Arylazetidines with Arylboronic Acids. <i>Advanced Synthesis and Catalysis</i> , 2021, 363, 2796-2805.	2.1	6
7	Siloxy Esters as Traceless Activators of Carboxylic Acids: Boron-Catalyzed Chemoselective Asymmetric Aldol Reaction**. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 24598-24604.	7.2	16
8	Experimental and Computational Studies on the Physicochemical Behavior of Phosphine Induced by Reactions with H and D Atoms on Interstellar Ice Grains. <i>Astrophysical Journal</i> , 2021, 918, 73.	1.6	9
9	Delivery of Electrons by Proton-Hole Transfer in Ice at 10 K: Role of Surface OH Radicals. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 704-710.	2.1	6
10	CO release from Mn(μ -O)-based photoCORMs with single photons in the phototherapeutic region. <i>Chemical Communications</i> , 2021, 57, 1101-1104.	2.2	8
11	CH ₃ O Radical Binding on Hexagonal Water Ice and Amorphous Solid Water. <i>Journal of Physical Chemistry A</i> , 2021, 125, 387-393.	1.1	16
12	Successive H-atom Addition to Solid OCS on Compact Amorphous Solid Water. <i>Astrophysical Journal</i> , 2021, 922, 146.	1.6	10
13	Phosphorescence properties of anionic cyclometalated platinum(II) complexes with fluorine-substituted tridentate diphenylpyridine in the solid state. <i>Chemical Physics Letters</i> , 2020, 739, 137024.	1.2	5
14	Palladium-Catalyzed Regioselective and Stereospecific Ring-Opening Cross-Coupling of Aziridines: Experimental and Computational Studies. <i>Accounts of Chemical Research</i> , 2020, 53, 1686-1702.	7.6	48
15	Photostimulated desorption of OH radicals from amorphous solid water: Evidence for the interaction of visible light with an OH-ice complex. <i>Physical Review A</i> , 2020, 102, .	1.0	15
16	A dinuclear Mo ₂ H ₈ complex supported by bulky C ₅ H ₂ tBu ₃ ligands. <i>Chemical Communications</i> , 2020, 56, 8035-8038.	2.2	7
17	Synthesis of Dinuclear Mo ^{IV} -Fe Hydride Complexes and Catalytic Silylation of N ₂ . <i>Chemistry - A European Journal</i> , 2020, 26, 9537-9546.	1.7	13
18	Bright Luminescent Platinum(II)-Biaryl Emitters Synthesized Without Air-Sensitive Reagents. <i>Chemistry - A European Journal</i> , 2020, 26, 5449-5458.	1.7	8

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19	Entropic corrections for the evaluation of the catalytic activity in the Al(η^5 -indenyl) η^5 -indenyl catalysed formation of cyclic carbonates from CO ₂ and epoxides. <i>Catalysis Science and Technology</i> , 2019, 9, 5433-5440.	2.1	11
20	Insight into the Origin of Competitive Emission of Copper(I) Complexes Bearing Diimine and Diphosphine Ligands. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 1684-1693.	2.0	12
21	Ultraviolet-photon exposure stimulates negative current conductivity in amorphous ice below 50 K. <i>Chemical Physics Letters</i> , 2019, 737, 136820.	1.2	6
22	Asymmetric Synthesis of α -Aryl Amino Acids through Pd-Catalyzed Enantiospecific and Regioselective Ring-Opening Suzuki-Miyaura Arylation of Aziridine-2-carboxylates. <i>Chemistry - A European Journal</i> , 2019, 25, 10226-10231.	1.7	14
23	Computational Study on the Mechanism and Origin of the Regioselectivity and Stereospecificity in Pd/SIPr-Catalyzed Ring-Opening Cross-Coupling of 2-Arylaziridines with Arylboronic Acids. <i>ACS Catalysis</i> , 2019, 9, 4582-4592.	5.5	12
24	Robust Triplatinum Redox-Chromophore for a Post-Synthetic Color-Tunable Electrochromic System. <i>Chemistry - A European Journal</i> , 2019, 25, 7669-7678.	1.7	9
25	A Luminescent Manganese PhotoCORM for CO Delivery to Cellular Targets under the Control of Visible Light. <i>Inorganic Chemistry</i> , 2018, 57, 1766-1773.	1.9	58
26	Predicting Reaction Pathways from Reactants. , 2018, , 321-349.		3
27	Luminescent ionic liquids based on cyclometalated platinum(η^5 -indenyl) complexes exhibiting thermochromic behaviour in different colour regions. <i>Dalton Transactions</i> , 2018, 47, 5589-5594.	1.6	22
28	Antimicrobial silver (I) complexes derived from aryl-benzothiazoles as turn-on sensors: Syntheses, properties and density functional studies. <i>Inorganica Chimica Acta</i> , 2018, 471, 326-335.	1.2	14
29	Titelbild: Measuring the Relative Reactivity of the Carbon-Hydrogen Bonds of Alkanes as Nucleophiles (<i>Angew. Chem.</i> 42/2018). <i>Angewandte Chemie</i> , 2018, 130, 13885-13885.	1.6	0
30	Measuring the Relative Reactivity of the Carbon-Hydrogen Bonds of Alkanes as Nucleophiles. <i>Angewandte Chemie</i> , 2018, 130, 14044-14048.	1.6	12
31	Phosphorescence Properties of Discrete Platinum(II) Complex Anions Bearing N-Heterocyclic Carbenes in the Solid State. <i>Inorganic Chemistry</i> , 2018, 57, 14086-14096.	1.9	34
32	Cubane-Type [Mo ₃ S ₄ M] Clusters with First-Row Groups...4-10 Transition-Metal Halides Supported by C ₅ Me ₅ Ligands on Molybdenum. <i>Chemistry - A European Journal</i> , 2018, 24, 17138-17147.	1.7	18
33	Measuring the Relative Reactivity of the Carbon-Hydrogen Bonds of Alkanes as Nucleophiles. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 13848-13852.	7.2	40
34	Solvent-Free Thermal Synthesis of Luminescent Dinuclear Cu(I) Complexes with Triarylphosphines. <i>Inorganic Chemistry</i> , 2018, 57, 5929-5938.	1.9	21
35	Expanding the Range of Force Fields Available for ONIOM Calculations: The SICTWO Interface. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1828-1835.	2.5	18
36	Functional-Group-Tolerant, Silver-Catalyzed N-N Bond Formation by Nitrene Transfer to Amines. <i>Journal of the American Chemical Society</i> , 2017, 139, 2216-2223.	6.6	62

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37	Luminescent Re(I) Carbonyl Complexes as Trackable PhotoCORMs for CO delivery to Cellular Targets. <i>Inorganic Chemistry</i> , 2017, 56, 2863-2873.	1.9	70
38	Development of Ion-Conductive and Vapoluminescent Porous Coordination Polymers Composed of Ruthenium(II) Metalloligand. <i>Inorganic Chemistry</i> , 2017, 56, 3005-3013.	1.9	19
39	Theoretical Study of Addition Reactions of L_4M ($M = Rh, Ir$) and L_2M ($M = Pd$) Tj ETQq1 1,0,784314,rgBT /O	1.1	5
40	DFT and AFIR Study on the Mechanism and the Origin of Enantioselectivity in Iron-Catalyzed Cross-Coupling Reactions. <i>Journal of the American Chemical Society</i> , 2017, 139, 16117-16125.	6.6	74
41	ONIOM(QM:AMOEBA09) Study on Binding Energies and Binding Preference of OH, HCO, and CH_3 Radicals on Hexagonal Water Ice (I_h). <i>Journal of Physical Chemistry C</i> , 2017, 121, 15223-15232.	1.5	19
42	Copper-Catalyzed Enantioselective Boron Conjugate Addition: DFT and AFIR Study on Different Selectivities of Cu(I) and Cu(II) Catalysts. <i>ACS Catalysis</i> , 2017, 7, 5370-5380.	5.5	28
43	DFT Rationalization of the Diverse Outcomes of the Iodine(III)-Mediated Oxidative Amination of Alkenes. <i>Chemistry - A European Journal</i> , 2016, 22, 7545-7553.	1.7	32
44	$Co_6H_8(P^i)_3$: A Cobalt Octahedron with Face-Capping Hydrides. <i>Angewandte Chemie</i> , 2016, 128, 16053-16057.	1.6	16
45	Computational Catalysis Using the Artificial Force Induced Reaction Method. <i>Accounts of Chemical Research</i> , 2016, 49, 763-773.	7.6	112
46	Artificial Force Induced Reaction Method for Systematic Determination of Complex Reaction Mechanisms. <i>Chemical Record</i> , 2016, 16, 2349-2363.	2.9	17
47	Dehydration of Methanediol in Aqueous Solution: An ONIOM(QM/MM) Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 6670-6676.	1.1	13
48	$Co_6H_8(P^i)_3$: A Cobalt Octahedron with Face-Capping Hydrides. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 15821-15825.	7.2	29
49	Computational Study of the Interactions between Benzene and Crystalline Ice I_h : Ground and Excited States. <i>ChemPhysChem</i> , 2016, 17, 4079-4089.	1.0	5
50	Palladium-catalyzed regioselective and stereo-invertive ring-opening borylation of 2-arylaziridines with bis(pinacolato)diboron: experimental and computational studies. <i>Chemical Science</i> , 2016, 7, 6141-6152.	3.7	69
51	Highly Twisted N,N -Dialkylamines as a Design Strategy to Tune Simple Aromatic Hydrocarbons as Steric Environment-Sensitive Fluorophores. <i>Journal of the American Chemical Society</i> , 2016, 138, 8194-8206.	6.6	135
52	The ONIOM Method and Its Applications. <i>Chemical Reviews</i> , 2015, 115, 5678-5796.	23.0	936
53	The Mechanism of Iron(II)-Catalyzed Asymmetric Mukaiyama Aldol Reaction in Aqueous Media: Density Functional Theory and Artificial Force-Induced Reaction Study. <i>Journal of the American Chemical Society</i> , 2015, 137, 11085-11094.	6.6	41
54	A computational view on the reactions of hydrocarbons with coinage metal complexes. <i>Journal of Organometallic Chemistry</i> , 2015, 784, 2-12.	0.8	39

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55	Double exchange in a mixed-valent octanuclear iron cluster, $[\text{Fe}_{8}(\mu_4\text{-O})_4(\mu_4\text{-4-Cl-pz})_{12}\text{Cl}_4]^{\cdot+}$. Dalton Transactions, 2014, 43, 11269-11276.	1.6	11
56	Chemo-, Regio-, and Stereoselective Silver-Catalyzed Aziridination of Dienes: Scope, Mechanistic Studies, and Ring-Opening Reactions. Journal of the American Chemical Society, 2014, 136, 5342-5350.	6.6	89
57	Catalytic cross-coupling of diazo compounds with coinage metal-based catalysts: an experimental and theoretical study. Dalton Transactions, 2013, 42, 4132.	1.6	57
58	A General Mechanism for the Copper- and Silver-Catalyzed Olefin Aziridination Reactions: Concomitant Involvement of the Singlet and Triplet Pathways. Journal of the American Chemical Society, 2013, 135, 1338-1348.	6.6	160
59	Attenuation of Conductance in Cobalt Extended Metal Atom Chains. Journal of Physical Chemistry C, 2012, 116, 20163-20172.	1.5	14
60	A Hierarchy of Methods for the Energetically Accurate Modeling of Isomerism in Monosaccharides. Journal of Chemical Theory and Computation, 2012, 8, 2630-2645.	2.3	52
61	Transition metal catalysis by density functional theory and density functional theory/molecular mechanics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 375-385.	6.2	91
62	A Combined Experimental and Computational Study of the Magnetic Superexchange within a Triangular $(\mu_3\text{-O})$ -Pyrazolato- FeIII_3 Complex. European Journal of Inorganic Chemistry, 2012, 2012, 3500-3506.	1.0	15
63	Mechanistic and Computational Studies of the Atom Transfer Radical Addition of CCl_4 to Styrene Catalyzed by Copper Homoscorpionate Complexes. Inorganic Chemistry, 2011, 50, 2458-2467.	1.9	36
64	Experimental and Theoretical Mössbauer Study of an Extended Family of $[\text{Fe}_8(\mu_4\text{-O})_4(\mu_4\text{-4-R-pz})_{12}\text{X}_4]$ Clusters. Inorganic Chemistry, 2011, 50, 1021-1029.	1.9	18
65	Quantum mechanics/molecular mechanics methods can be more accurate than full quantum mechanics in systems involving dispersion correlations. Physical Chemistry Chemical Physics, 2011, 13, 10520.	1.3	18
66	On the mechanism of water oxidation by a bimetallic manganese catalyst: A density functional study. Dalton Transactions, 2011, 40, 3859.	1.6	44
67	On the oxidation of alkyl and aryl sulfides by $[(\text{Me}_3\text{TACN})\text{MnVO}(\text{OH})_2]^+$: A density functional study. Inorganica Chimica Acta, 2008, 361, 1079-1086.	1.2	11
68	The role of substrate in unmasking oxyl character in oxomanganese complexes: the key to selectivity?. Dalton Transactions, 2008, , 6141.	1.6	22
69	Polysaccharides in Solution: Experimental and Computational Studies. , 0, , .		9
70	Siloxy Esters as Traceless Activators of Carboxylic Acids: Boron-Catalyzed Chemoselective Asymmetric Aldol Reaction. Angewandte Chemie, 0, , .	1.6	6