1.	Rational design of novel N-doped polyaromatic hydrocarbons as	2020
	donors for the perylene based dye-sensitized solar cells	
	M Karuppusamy, VSK Choutipalli, D Vijay, V Subramanian	
	Journal of Chemical Sciences 132 (1), 20	0000
2.	,	2020
	n= 1–6) clusters: a comparison of hybrid DFT with MP2/CBS and	
	CCSD (T)/CBS methods	
	KR Maiyelvaganan, MK Ravva, M Prakash, V Subramanian	
3.	Theoretical Chemistry Accounts 139 (9), 1-14 Electrocatalytic Reduction of CO ₂ to Ethylene by Molecular Cu-	2020
٦.	Complex Immobilized on Graphitized Mesoporous Carbon	2020
	M Balamurugan, HY Jeong, VSK Choutipalli, JS Hong, H Seo,	
	Small, 2000955	
4.	Bifunctional Electrocatalytic Activity of Ordered Intermetallics Based	2020
	on Pd and Sn	
	S Mondal, VSK Choutipalli, BK Jena, V Subramanian, CR Raj	
	The Journal of Physical Chemistry C 124 (18), 9631-9643	
5.		2020
	Based D-π-A Dyes: Leads from DFT Calculations	
	R Venkatraman, SVK Panneer, E Varathan, V Subramanian	
-	The Journal of Physical Chemistry A 124 (17), 3374-3385	2020
ь.	Leveraging columnar encoding for query operations	2020
	H Li, A Amor, S Subramanian, CC Lin, V Subramanian US Patent 10,572,475	
7.	Conveniently Synthesized Butterfly-Shaped Bitriphenylenes and their	2020
, ,	Application in Solution-Processed Organic Field-Effect Transistor	
	Devices	
	J Ramakrishna, L Karunakaran, SVK Paneer, AM Chennamkulam,	
	European Journal of Organic Chemistry 2020 (6), 662-673	
8.	Performance of Force-Field-and Machine Learning-Based Scoring	2020
	Functions in Ranking MAO-B Protein–Inhibitor Complexes in	
	Relevance to Developing Parkinson's Therapeutics	
	NA Murugan, C Muvva, C Jeyarajpandian, J Jeyakanthan,	
	International journal of molecular sciences 21 (20), 7648	0000
9.	Multipolar triphenylamines: Effect of spectator donor-acceptor pair on	2020
	intramolecular charge transfer interactions	
	P Thamaraiselvi, E Varathan, V Subramanian, S Easwaramoorthi Dyes and Pigments 172, 107838	
10	Role of Graphitic Nitrogen and π-Conjugated Functional Groups in	2019
	Selective Oxidation of Alcohols: A DFT based Mechanistic Elucidation	
	VS Kumar Choutipalli, V Subramanian	
	Chemistry–An Asian Journal 14 (24), 4798-4806	
11	Mechanistic Elucidation of the Structure and Reactivity of Bare and	2019
	Hydride-Protected Ag ₁₇ ⁺ Clusters	
	A Baksi, M Jash, S Bag, SK Mudedla, M Bodiuzzaman, D Ghosh,	
	The Journal of Physical Chemistry C 123 (46), 28494-28501	
12	Hydrogen bonding interaction of N5H with water: A first principle	2019
	calculations	
	R Pawar, V Subramanian	
4.0	Computational and Theoretical Chemistry 1165, 112560	2040
13	Unraveling the Unbinding Pathways of Products Formed in Catalytic	2019
	Reactions Involved in SIRT1–3: A Random Acceleration Molecular	
	Dynamics Simulation Study	
	C Muvva, NA Murugan, VS Kumar Choutipalli, V Subramanian	<u> </u>

	Journal of chemical information and modeling 59 (10), 4100-4115	
14	Interactions of thiol and alkoxy radical with coinage metal	2019
	nanoclusters	
	S Haseena, RM Kumar, V Rajapandian, V Subramanian	
	Applied Surface Science 487, 1409-1419	
15	Conformational Changes of Protein upon Encapsulation of Noble	2019
	Metal Clusters: An Investigation by Hydrogen/Deuterium Exchange	
	Mass Spectrometry	
	D Ghosh, SK Mudedla, MR Islam, V Subramanian, T Pradeep	
	The Journal of Physical Chemistry C 123 (28), 17598-17605	
16	Storage formats for in-memory caches	2019
	A Mishra, SK Chavan, V Subramanian, ESC Soylemez, A Kociubes,	
	US Patent App. 15/943,335	
17	Theoretical insights into the role of water molecules in the	2019
	guanidinium-based protein denaturation process in specific to	
	aromatic amino acids	
	K Balamurugan, M Prakash, V Subramanian	
	The Journal of Physical Chemistry B 123 (10), 2191-2202	
18	Mechanistic Elucidation of the Structure and Reactivity of Bare and	2019
	Hydride-Protected Ag ₁₇ ⁺ Clusters	
	A Baksi, M Jash, S Bag, SK Mudedla, M Bodiuzzaman, D Ghosh,	
19	Achieving highly efficient CO 2 to CO electroreduction exceeding 300	2019
	mA cm- 2 with single-atom nickel electrocatalysts	
	HY Jeong, M Balamurugan, VSK Choutipalli, E Jeong, V Subramanian,	
	Journal of Materials Chemistry A 7 (17), 10651-10661	
20	Destabilization of amyloid fibrils on interaction with MoS 2-based	2019
	nanomaterials	
	SK Mudedla, NA Murugan, V Subramanian, H Agren	
	RSC advances 9 (3), 1613-1624	2040
21	Excited state C–N bond dissociation and cyclization of tri-aryl amine-	2019
	based OLED materials: a theoretical investigation	
	V Subramanian, B Rajakumar Physical Chamieta Chamical Physics 31 (1) 438 447	
22	Physical Chemistry Chemical Physics 21 (1), 438-447	2019
22	Superprismane: A porous carbon allotrope NVR Nulakani, V Subramanian	2019
	Chemical Physics Letters 715, 29-33	
23	Frontispiece: Tris(2-benzimidazolylmethyl)amine-Directed Synthesis	2018
23	of Single-Atom Nickel Catalysts for Electrochemical CO Production	
	from CO ₂	
	HY Jeong, M Balamurugan, VSK Choutipalli, J Jo, H Baik, V Subramanian,	
	Chemistry–A European Journal 24 (69)	
2/	Tris(2-benzimidazolylmethyl)amine-Directed Synthesis of Single-Atom	2018
27	Nickel Catalysts for Electrochemical CO Production from CO ₂	20.0
	HY Jeong, M Balamurugan, VSK Choutipalli, J Jo, H Baik, V Subramanian,	
	Chemistry–A European Journal 24 (69), 18444-18454	
25	Water catalyzed pyrolysis of oxygen functional groups of coal: A	2018
23	density functional theory investigation	
	SK Mudedla, CVS Kumar, A Suresh, P Baskar, PS Dash, V Subramanian	
	Fuel 233, 328-335	
26	Design, synthesis and photophysical investigation of triphenylamine-	2018
20	bithiophene dyes as RGB emitters for white light applications	
	A Krishna, E Varathan, P Sreedevi, V Subramanian, V Karunakaran,	
	Transma, - varaman, r. Sissasti, v. Sastamanian, v. Naramanani, m.	1

27	Reply to the Comment on "Michael Addition Based Chemodosimeter for Serum Creatinine Detection Using (<i>E</i>)-3-(Pyren-2-yl)-1-(3,4,5-trimethoxyphenyl)prop-2-en E Sundaram, V Subramanian, K Velayutham, R Gomathinayagam,	2018
	ACS sensors 3 (11), 2467-2470	
28	Experimental and Theoretical Investigations of Different Diketopyrrolopyrrole-Based Polymers P Murugan, V Raghavendra, S Chithiravel, K Krishnamoorthy, AB Mandal, ACS omega 3 (9), 11710-11717	2018
29	Co-operativity in non-covalent interactions in ternary complexes: a comprehensive electronic structure theory based investigation SVK Panneer, MK Ravva, BK Mishra, V Subramanian, N Sathyamurthy Journal of Molecular Modeling 24 (9), 258	2018
30	Exploring multifunctional applications of hexagonal boron arsenide sheet: a DFT study K Manoharan, V Subramanian ACS omega 3 (8), 9533-9543	2018
31	Bent Keto Form of Curcumin, Preferential Stabilization of Enol by Piperine, and Isomers of Curcumin∩ Cyclodextrin Complexes: Insights from Ion Mobility Mass Spectrometry A Nag, P Chakraborty, G Natarajan, A Baksi, SK Mudedla, Analytical chemistry 90 (15), 8776-8784	2018
32	Guanidinium cation—water clusters M Prakash, T Vanidasan, V Subramanian Theoretical Chemistry Accounts 137 (7), 108	2018
33	Michael Addition Based Chemodosimeter for Serum Creatinine Detection Using (<i>E</i>)-3-(Pyren-2-yl)-1-(3,4,5-trimethoxyphenyl)prop-2- en-1-one Chalcone E Sundaram, V Subramanian, K Velayutham, R Gomathinayagam, ACS sensors 3 (4), 763-771	2018
34	Design and synthesis of novel polyamine collector to recover iron values from iron ore slimes AS Patra, NVR Nulakani, YP Kumar, V Subramanian, J Dash, Powder Technology 325, 180-191	2018
35	Probing the effect of different graphitic nitrogen sites on the aerobic oxidation of thiols to disulfides: a DFT study. JS Vijaya, M Kamaraj, V Subramanian Physical chemistry chemical physics: PCCP 20 (3), 2057-2065	2018
36	Two-acceptor one-donor random terpolymers comprising thiophene- and phenyl-capped diketopyrrolopyrrole for organic photovoltaics B Sambathkumar, E Varathan, V Subramanian, N Somanathan New Journal of Chemistry 42 (24), 20113-20122	2018
37	Design, Synthesis and Photophysical Investigation of Triphenylamine-bithiophene Dyes as RGB Emitters For White Light Applications K Venugopal, P Sreedevi, V Subramanian, A Krishna, R Luxmi Varma, Elsevier	2018
38	Computational realization of Dirac nodal point and Dirac nodal loop fermions in novel β-graphyne analogues NVR Nulakani, V Subramanian Journal of Materials Chemistry C 6 (28), 7626-7634	2018
39	Understanding proton capture and cation-induced dimerization of [Ag 29 (BDT) 12] 3- clusters by ion mobility mass spectrometry P Chakraborty, A Baksi, SK Mudedla, A Nag, G Paramasivam, Physical Chemistry Chemical Physics 20 (11), 7593-7603	2018

		2040
40	Carbon flakes based metal organic frameworks for H 2, CH 4 and CO	2018
	2 gas storage: a GCMC simulation study	
	K Gopalsamy, V Subramanian	
	New Journal of Chemistry 42 (6), 4240-4250	
41	Triphenylamine based yellowish-orange light emitting organic dyes	2018
	(donor-π-acceptor) for hybrid WLEDs and OLEDs: synthesis,	
	characterization and theoretical study	
	AB Kajjam, PSV Kumar, V Subramanian, S Vaidyanathan	
	Physical Chemistry Chemical Physics 20 (6), 4490-4501	
12	Probing the effect of different graphitic nitrogen sites on the aerobic	2018
42	• • • • • • • • • • • • • • • • • • • •	2010
	oxidation of thiols to disulfides: a DFT study	
	JV Sundar, M Kamaraj, V Subramanian	
42	Physical Chemistry Chemical Physics 20 (3), 2057-2065	2017
43	Cp-Graphyne: a low-energy graphyne polymorph with double	2017
	distorted Dirac points	
	NVR Nulakani, V Subramanian	
	ACS omega 2 (10), 6822-6830	
44	Stereoselective Palladium-Catalyzed Synthesis of Indolines via	2017
	Intramolecular Trapping of N-Ylides with Alkenes	
	ACS Reddy, VSK Choutipalli, J Ghorai, V Subramanian, P Anbarasan	
	ACS Catalysis 7 (9), 6283-6288	
45	Au ₂₂ Ir ₃ (PET) ₁₈ : An Unusual Alloy Cluster through Intercluster	2017
73	Reaction	
	S Bhat, A Baksi, SK Mudedla, G Natarajan, V Subramanian, T Pradeep	
4.0	The Journal of Physical Chemistry Letters 8 (13), 2787-2793	2017
46	Nanoclusters of Cyanuric Acid	2017
	M Elango, V Subramanian, N Sathyamurthy	
	Journal of Chemical Sciences 129 (7), 873-881	0047
47	Gold-induced unfolding of lysozyme: toward the formation of	2017
	luminescent clusters	
	D Ghosh, A Baksi, SK Mudedla, A Nag, MA Ganayee, V Subramanian,	
	The Journal of Physical Chemistry C 121 (24), 13335-13344	
48	Isomerism in monolayer protected silver cluster ions: an ion mobility-	2017
	mass spectrometry approach	
	A Baksi, A Ghosh, SK Mudedla, P Chakraborty, S Bhat, B Mondal,	
	The Journal of Physical Chemistry C 121 (24), 13421-13427	
49	Assessing therapeutic potential of molecules: molecular property	2017
	diagnostic suite for tuberculosis	
	AS Gaur, A Bhardwaj, A Sharma, L John, MR Vivek, N Tripathi,	
	Journal of Chemical Sciences 129 (5), 515-531	2017
50	Can boron antisites of BNNTs be an efficient metal-free catalyst for	2017
	nitrogen fixation?—A DFT investigation	
	CVS Kumar, V Subramanian	
	Physical Chemistry Chemical Physics 19 (23), 15377-15387	
51	The role of sulfur oxidation in controlling the electronic properties of	2017
	sulfur-containing host molecules for phosphorescent organic light-	
	emitting diodes	
	E Varathan, V Subramanian	
1	Physical Chemistry Chemical Physics 19 (19), 12002-12012	
בי	Highly clean and efficient enzymatic dehairing in green solvents	2017
32		2017
	R Aravindhan, V Monika, K Balamurugan, V Subramanian, JR Rao,	
	Journal of Cleaner Production 140, 1578-1586	2047
53	Quantitative structure-activity/property/toxicity relationships through	2017
	conceptual density functional theory-based reactivity descriptors	

	S Pan, AK Gupta, V Subramanian, PK Chattaraj	
	Pharmaceutical Sciences: Breakthroughs in Research and Practice, 1517-1572	
54	Unravelling the Structural Changes in α-Helical Peptides on	2016
	Interaction with Convex, Concave, and Planar Surfaces of Boron-	
	Nitride-Based Nanomaterials	
	SK Mudedla, K Balamurugan, V Subramanian	
	The Journal of Physical Chemistry C 120 (49), 28246-28260	
55	Ab initio and density functional theory (DFT) studies on triflic acid with	2016
	water and protonated water clusters	
	M Prakash, V Subramanian	
	Journal of molecular modeling 22 (12), 293	
56	Two Donor–One Acceptor Random Terpolymer Comprised of	2016
	Diketopyrrolopyrrole Quaterthiophene with Various Donor π-Linkers	
	for Organic Photovoltaic Application	
	B SambathKumar, P Shyam Vinod Kumar, FS Deepakrao, SS Kumar Iyer,	
	The Journal of Physical Chemistry C 120 (47), 26609-26619	
57	Bader's theory of atoms in molecules (AIM) and its applications to	2016
37	, , , , , , , , , , , , , , , , , , , ,	2010
	chemical bonding	
	PSV Kumar, V Raghavendra, V Subramanian Journal of Chemical Sciences 128 (10), 1527-1536	
ГО		2016
56	One hundred years of Lewis Chemical Bond! E Arunan, ED Jemmis, V Subramanian	2010
	Journal of Chemical Sciences 128 (10), 1517-1518	
ΕO		2016
39	Role of alkaline earth metal cations in improving the hydrogen-	2010
	storage capacity of polyhydroxy adamantane: a DFT study	
	K Gopalsamy, V Subramanian The Journal of Physical Chemistry C 130 (36) 10033 10041	
60	The Journal of Physical Chemistry C 120 (36), 19932-19941 Theoretical Design of Represelent discrete Person Organic Departments of Physical Chemistry C 120 (186), 19932-19941	2016
60	Theoretical Design of Benzoselenadiazole Based Organic Donor	2010
	Molecules for Solar Cell Applications	
	PSV Kumar, E Varathan, D Vijay, V Subramanian	
C1	Proceedings of the National Academy of Sciences, India Section A: Physical	2016
91	Identification of an electrostatic ruler motif for sequence-specific	2010
	binding of collagenase to collagen	
	SR Subramanian, ERA Singam, M Berinski, V Subramanian, RC Wade	
	The Journal of Physical Chemistry B 120 (33), 8580-8589	2010
62	MMpI: A WideRange of Available Compounds of Matrix	2016
	Metalloproteinase Inhibitors	
	C Muvva, S Patra, S Venkatesan	
	Plos one 11 (8), e0159321	0040
63	A theoretical study on the design, structure, and electronic properties	2016
	of novel forms of graphynes	
	NVR Nulakani, V Subramanian	
	The Journal of Physical Chemistry C 120 (28), 15153-15161	0010
64	A highly selective chemosensor for cyanide derived from a formyl-	2016
	functionalized phosphorescent iridium (III) complex	
	KS Bejoymohandas, A Kumar, S Sreenadh, E Varathan, S Varughese,	
	Inorganic Chemistry 55 (7), 3448-3461	
65	Application of Conceptual Density Functional Theory in Developing	2016
	QSAR Models and their Usefulness in the Prediction of Biological	
	Activity and Toxicity of Molecules	
	S Pan, A Gupta, D Roy, R Sharma, V Subramanian, A Mitra, P Chattaraj	
	Chemometrics Applications and Research: QSAR in Medicinal Chemistry, 183-214	
66	Overview and Recent Advances in QSAR Studies	2016
	RP Gangwal, MV Damre, AT Sangamwar	

		1
	Chemometrics Applications and Research: QSAR in Medicinal Chemistry, 1	0040
67	Stereo-, Regio-, and Chemoselective $[3 + 2]$ -Cycloaddition of $(2E, 4E)$ -	2016
	Ethyl 5-(Phenylsulfonyl)penta-2,4-dienoate with Various Azomethine	
	Ylides, Nitrones, and	
	U Sankar, CV Surya Kumar, V Subramanian, KK Balasubramanian, The Journal of Organic Chemistry 81 (6), 2340-2354	
68	Dioxin sensing properties of graphene and hexagonal boron nitride	2016
	based van der Waals solids: a first-principles study	
	M Kamaraj, JV Sundar, V Subramanian	
	RSC advances 6 (108), 107114-107126	
69	White electroluminescence from a single polymer system:	2016
	phenothiazine derivatives as a red emissive dopant and polyfluorene	
	as a blue host	
	S Nagaraju, E Ravindran, E Varathan, V Subramanian, N Somanathan RSC advances 6 (95), 92778-92785	
70	Self-assembly of a white-light emitting polymer with aggregation	2016
	induced emission enhancement using simplified derivatives of	
	tetraphenylethylene	
	E Ravindran, E Varathan, V Subramanian, N Somanathan	
	Journal of Materials Chemistry C 4 (34), 8027-8040	
71	Quantum chemical design of carbazole-and pyridoindole-based	2016
	ambipolar host materials for blue phosphorescent OLEDs	
	E Varathan, D Vijay, V Subramanian	
	RSC advances 6 (78), 74769-74784	0040
72	Structure-properties relationship in diketopyrrolopyrrole based small	2016
	molecules using functional terminal side chains via direct arylation: a	
	joint experimental and theoretical	
	B Sambathkumar, P Shyam Vinod Kumar, K Saurav, S Sundar Kumar Iyer,	
72	New Journal of Chemistry Photophysical and charge transport properties of pyrazolines	2016
/3	J Ajantha, E Varathan, V Bharti, V Subramanian, S Easwaramoorthi,	2010
	RSC advances 6 (1), 786-795	
74	Design of medium band gap random terpolymers containing fluorene	2016
	linked diketopyrrolopyrrole and thiophene co-monomers: an	
	experimental and theoretical study	
	B SambathKumar, E Varathan, V Subramanian, N Somanathan	
	New Journal of Chemistry 40 (2), 1377-1386	
75	Interaction of nucleobases with silicon doped and defective silicon	2016
	doped graphene and optical properties	
	SK Mudedla, K Balamurugan, M Kamaraj, V Subramanian	
	Physical Chemistry Chemical Physics 18 (1), 295-309	0045
/6	Generalized reaction mechanism for the selective aerobic oxidation of	2015
	aryl and alkyl alcohols over nitrogen-doped graphene	
	VS Jeyaraj, M Kamaraj, V Subramanian The Journal of Physical Chemistry C 119 (47), 26438-26450	
77	Theoretical insights into the role of water in the dissolution of cellulose	2015
,,	using IL/water mixed solvent systems	20.0
	R Parthasarathi, K Balamurugan, J Shi, V Subramanian, BA Simmons,	
	The Journal of Physical Chemistry B 119 (45), 14339-14349	
78	AntiAngioPred: a server for prediction of anti-angiogenic peptides	2015
	ASE Ramaprasad, S Singh, S Venkatesan	
	PloS one 10 (9), e0136990	
79	Effect of graphene oxide on the conformational transitions of amyloid	2015
	beta peptide: A molecular dynamics simulation study	<u> </u>

	L Baweja, K Balamurugan, V Subramanian, A Dhawan Journal of Molecular Graphics and Modelling 61, 175-185	
80	A new class of MPV type reduction in group 4 alkoxide complexes of salicylaldiminato ligands: Efficient catalysts for the ROP of lactides, epoxides and polymerization of ethylene	2015
	D Chakraborty, D Mandal, V Ramkumar, V Subramanian, JV Sundar Polymer 56, 157-170	
81	Enhancement of internal motions of lysozyme through interaction with gold nanoclusters and its optical imaging SK Mudedla, ERA Singam, J Vijay Sundar, MN Pedersen, NA Murugan, The Journal of Physical Chemistry C 119 (1), 653-664	2015
82	Influence of the size and charge of gold nanoclusters on complexation with siRNA: a molecular dynamics simulation study SK Mudedla, ERA Singam, K Balamurugan, V Subramanian Physical Chemistry Chemical Physics 17 (45), 30307-30317	2015
83	Coro-graphene and circumcoro-graphyne: novel two-dimensional materials with exciting electronic properties NVR Nulakani, M Kamaraj, V Subramanian RSC advances 5 (96), 78910-78916	2015
84	Adsorption of guanidinium collectors on aluminosilicate minerals—a density functional study NVR Nulakani, P Baskar, AS Patra, V Subramanian Physical Chemistry Chemical Physics 17 (37), 23805-23815	2015
85	Photophysical and electroluminescence properties of bis (2', 6'-difluoro-2, 3'-bipyridinato-N, C 4') iridium (picolinate) complexes: effect of electron-withdrawing and KS Bejoymohandas, A Kumar, S Varughese, E Varathan, V Subramanian, Journal of Materials Chemistry C 3 (28), 7405-7420	2015
86	Design and synthesis of sugar-triazole based uracil appended sugar- imine derivatives—an application in DNA binding studies A Hemamalini, ERA Singam, SK Mudedla, V Subramanian, TM Das New Journal of Chemistry 39 (6), 4575-4582	2015
87	White light emitting single polymer from aggregation enhanced emission: a strategy through supramolecular assembly E Ravindran, SJ Ananthakrishnan, E Varathan, V Subramanian, Journal of Materials Chemistry C 3 (17), 4359-4371	2015
88	Design, synthesis and metal sensing studies of ether-linked bistriazole derivatives A Hemamalini, SK Mudedla, V Subramanian, TM Das New Journal of Chemistry 39 (5), 3777-3784	2015
89	Interaction of collagen like peptides with gold nanosurfaces: a molecular dynamics investigation R Gopalakrishnan, ERA Singam, JV Sundar, V Subramanian Physical Chemistry Chemical Physics 17 (7), 5172-5186	2015