

FORTHCOMING PAPERS (As on 5 June 2017)							
April issue is published							
Sr. No.	Issue	Publi shed ONLINE	Ref. No.	Title	Corresponding Author	Email ID	Date of acceptance
1	Special Issue - THEORETICAL CHEMISTRY/CHEMICAL DYNAMICS, July	YES	JCSC-D-16-01289R1	Modeling of 1-D Nanowires and Analyzing Their Hydrogen and Noble Gas Binding Ability	PK Chattaraj, Ph. D.	pkc@chem.iitkgp.ernet.in ;pratim.chattaraj@gmail.com	3-Jan
2	Special Issue - THEORETICAL CHEMISTRY/CHEMICAL DYNAMICS, July	YES	JCSC-D-16-01347	A model with charges and polarizability for CS ₂ in an ionic liquid	Ruth Lynden-Bell	rmlb@cam.ac.uk	4-Jan
3	Special Issue - THEORETICAL CHEMISTRY/CHEMICAL DYNAMICS, July	YES	JCSC-D-16-01314R1	Molecular Dynamics Investigation of Efficient SO ₂ Absorption by Anion-Functionalized Ionic Liquids'	S BALASUBRAMAN IAN	bala@jncasr.ac.in;jncbala@gmail.com	16-Jan
4	Special Issue - THEORETICAL CHEMISTRY/CHEMICAL	YES	JCSC-D-16-01281R1	Size and Structure of Cytochrome C bound to Gold nano-clusters: Effect of Ethanol'	K Bhattacharyya	kankan.bhattacharyya@gmail.com	20-Jan

	DYNAMICS, July						
5	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July	YES	JCSC-D-16- 01395R1	Breakdown of universal Lindemann criterion in the melting of Lennard-Jones polydisperse solids	Biman Bagchi	bbagchi@sscu.iisc.ernet.i n;profbiman@gmail.com	31-Jan
6	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-16- 01477R1	In Silico Studies of the Early Stages of Aggregation of A β ₄₂ Peptides	Sanjoy Bandyopadhyay	sanjoy@chem.iitkgp.ernet .in	8-Feb
7	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July	YES	JCSC-D-17- 00008R1	Validity of the Rosenfeld relationship: A comparative study of the network forming NTW model and other simple liquids.	Sarika Maitra Bhattacharyya, Ph D		8-Feb
8	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July	YES	JCSC-D-17- 00120	Trajectories of Brownian particles with space-correlated noise.	Edoardo Milotti	milotti@ts.infn.it	24-Feb

9	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July	YES	JCSC-D-16- 01370R1	Nanoclusters of cyanuric acid	Subramanian Venkatesan	subuchem@hotmail.com	3-Mar
10	May	YES	JCSC-D-16- 01363R2	Silver(I) and Copper(II)-Imidazolium Carboxylates: Efficient Catalysts in Ullmann Coupling Reactions	Prabusankar Ganesan	prabu@iith.ac.in	9-Mar
11	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17- 00075R1	Density-scaling exponents and virial potential-energy correlation coefficients for the (2n,n) Lennard-Jones system	Jeppe Dyre	dyre@ruc.dk	9-Mar
12	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17- 00109R1	Microstructures and Their Lifetimes in Acetamide/Electrolyte Deep Eutectics: Anion Dependence	Ranjit Biswas	ranjit@bose.res.in	12-Mar
13	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17- 00129R1	Comparison of Coarse-grained (MARTINI) and Atomistic Molecular Dynamics Simulations of alpha and beta Toxin Nanopores in Lipid Membranes	K Ganapathy Ayappa	ayappa@chemeng.iisc.ernet.in	15-Mar

14	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17- 00028R1	Stabilisation of the [6]-prismane structure by silicon substitution'	N Sathyamurthy	nsath@iitk.ac.in;nsath@ii sermohali.ac.in	17-Mar
15	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17- 00208	Vibrational Echo Spectral Observables and Frequency Fluctuations of Hydration Shell Water around a Fluoride Ion from First Principles Simulations'	A Chandra	amalen@iitk.ac.in	20-Mar
16	May	YES	JCSC-D-17- 00093R1	Bis(Pyrrole-benzimidazole) conjugates as novel colorimetric sensor for anions'	Sanjeev Pran Mahanta	samahanta@gmail.com;sp m@tezu.ernet.in	21-Mar
17	May	YES	JCSC-D-17- 00268R1	Assessing Therapeutic Potential of Molecules: Molecular Property Diagnostic Suite for Tuberculosis (MPDSTB)'	G N Sastry	gnsastry@gmail.com;gnsa stry@iict.res.in	22-Mar
18	May	YES	JCSC-D-16- 01333R1	Polyoxometalate-based 3D Porous Framework with Inorganic Molecular Nanocage Units'	Shaobin Li	qqhr1sb1022@126.com	22-Mar
19	May	YES	JCSC-D-17- 00110R1	On the Effect of External Perturbation on Amino Acid Salt Bridge: A DFT Study'	Pradip Kr. Bhattacharyya	prdpbhatta@yahoo.com	22-Mar
20	May	YES	JCSC-D-17- 00140R1	Inclusion complexation of tetrabutylammonium iodide by cyclodextrins'	Dr. Mahendra Nath Roy	mahendraroy2002@yaho o.co.in	24-Mar

21	May	YES	JCSC-D-17-00077R1	Synthesis and structural studies of half-sandwich Cp* rhodium and Cp* iridium complexes featuring mono, bi and tetradentate nitrogen and oxygen donor ligands'	Mohan Rao Kollipara	mohanrao59@gmail.com	26-Mar
22	May	YES	JCSC-D-16-01471R1	Ammonia treated Mo/AC catalysts for CO hydrogenation with an improved oxygenates selectivity'	Nagaraju Pasupulety	pasupulety@gmail.com	27-Mar
23	May	YES	JCSC-D-16-01334R3	Exploration of DNA Interactions and Biocidal activity of Incorporated Benzothiazole Schiff base complexes: Synthesis and validation'	SHIVA RAJ	shivaraj_sunny@yahoo.co.in	28-Mar
24	May	YES	JCSC-D-16-01088R1	Studies on dehydrogenation of cyclohexanol to cyclohexanone over mesoporous supported copper catalysts'	K S Rama Rao	ksramarao@iict.res.in;cat_symp_21@yahoo.com	28-Mar
25	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17-00108R1	A Free Energy Study of the Liquid-Liquid Phase Transition of the Jagla Two-ScalePotential'	Pablo Debenedetti	pdebene@princeton.edu	28-Mar
26	May	YES	JCSC-D-17-00015R1	Synthesis of novel bis-allyloxy and hydroxypropoxy derivatives of 4,5-diaryl thiophene-2-carboxylic acid and their biological evaluation'	<u>Shanmuganathan T</u>	t_shanmuganathan09@yahoo.com	2-Apr
27	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS,		JCSC-D-16-01426R1	Excess vibrational modes of a crystal in an external non-affine field'	Surajit Sengupta	surajit@tifrh.res.in	3-Apr

	July						
28	May	YES	JCSC-D-17-00234R2	Employment of different spectroscopic tools for the investigation of chromium (VI) oxidation of acetaldehyde in aqueous micellar medium'	Bidyut Saha	b_saha31@rediffmail.com	6-Apr
29	May	YES	JCSC-D-16-01290R2	Interaction energies and structures of the $\text{Li}^+(\text{CO})_n$ ($n = 1-3$) complexes'	Jamal Dawoud	jamaldawoud@hu.edu.jo	8-Apr
30	June	YES	JCSC-D-17-00063R1	Theoretical study on the Molecular Structure, Intermolecular interaction and Spectral Features of 2-Aminopyridine with 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone Complex'	hailong wang	wanghailong@mail.zjxu.edu.cn	8-Apr
31	June	YES	JCSC-D-16-01361R1	Synthesis, experimental and theoretical vibrational studies of 1-methyl and 1,2-dimethyl, 3-propyl imidazolium bis(trifluoromethanesulfonyl)imide'	Annalisa Paolone	annalisa.paolone@roma1.infn.it	11-Apr
32	June		JCSC-D-17-00133R1	Synthesis, Characterization, X-ray structure, optical properties and theoretical calculations of condensed phthalazines'	Abdelmalek Bouraiou	bouraiou.abdelmalek@yahoo.fr	11-Apr
33	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17-00125	Controlling the quantum rotational dynamics of a driven planar rotor by rebuilding barriers in the classical phase space'	Srihari Keshavamurthy	srihari@iitk.ac.in	11-Apr
34	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL		JCSC-D-17-00115R1	A comparative study of the performance of some density functionals for vibronic spectra	M Durga Prasad	mdpssc@uohyd.ac.in	13-Apr

	DYNAMICS, July						
35	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17- 00229R1	Density dependence of relaxation dynamics in glass formers, and the dependence of their fragility on the softness of inter-particle interactions'	Srikanth Sastry	sastry@jncasr.ac.in	14-Apr
36	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17- 00182	The dynamic behavior of the exohedral transition metal complexes of B40: η^6 - and η^7 -B40Cr(CO) ₃ and Cr(CO) ₃ - η^7 -B40- η^7 - Cr(CO) ₃ '	Eluvathingal D Jemmis	jemmis@ipc.iisc.ernet.in; jemmis@gmail.com	14-Apr
37	August		JCSC-D-17- 00329R1	N-(acyl)-N'-(ferrocenylidene)hydrazines and their nickel(II) complexes: Syntheses, structures and physical properties'	Samudranil Pal	spal@uohyd.ac.in	14-Apr
38	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July	YES	JCSC-D-17- 00144R1	Unfolding intermediates of the mutant His- 107-Tyr of human carbonic anhydrase II'	Srabani Taraphder	srabani@chem.iitkgp.ernet.in	17-Apr
39	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17- 00155R1	Role of Solvation Structure in the Shuttling of the Hydrated Excess Proton'	Greg Voth	gavoth@uchicago.edu	18-Apr

40	June	YES	JCSC-D-17-00271R1	An efficient domino one-pot synthesis of novel spirofuran-indenoquinoxalines by vinyltriphenylphosphonium salts'	Malek Taher Maghsoodlou	mt_maghsoodlou@yahoo.com	19-Apr
41	August		JCSC-D-17-00290R1	Cationic and Neutral Copper (I) Iodide Cluster MOFs derived from tridentate N-donor functionalized P(V) ligands: Synthesis, Structure and Photophysical Properties'	Boomishankar Ramamoorthy	boomi@iiserpune.ac.in	20-Apr
42	August		JCSC-D-17-00104R2	Theory for Electrochemical Impedance Spectroscopy of Heterogeneous Electrode with Distributed Capacitance and Charge Transfer Resistance'	Rama Kant	rkant@chemistry.du.ac.in	21-Apr
43	June		JCSC-D-17-00304R1	N ₂ ,N ₂ ,N ₄ ,N ₄ ,N ₆ ,N ₆ -hexa(1H-tetrazol-5-yl)-1,3,5-triazine-2,4,6-triamine as a nitrogen-rich material'	Krishnamurthi Muralidharan	kmsc@uohyd.ernet.in; murali@uohyd.ac.in	22-Apr
44	June		JCSC-D-16-00918R3	Synthesis and evaluation of aromaticity and tautomerization of pyrazolopyridazin(on)es'	Nurettin Menges	nurettinmenges@gmail.com	24-Apr
45	Special Issue - THEORETICAL CHEMISTRY/CHEMICAL DYNAMICS, July		JCSC-D-17-00124R1	A coarse-grained model based on core-softened potentials for anomalous polymers'	Marcia C. Barbosa	marcia.barbosa@ufrgs.br	24-Apr
46	Special Issue - THEORETICAL CHEMISTRY/CHEMICAL DYNAMICS, July		JCSC-D-17-00117R1	A molecular dynamics calculation of solid phase of malonic acid : Role of hydrogen-bond chains and the elastic constants'	S. Yashonath	yashonath@sscu.iisc.ernet.in; yashonath@gmail.com	1-May
47	Special Issue - THEORETICAL		JCSC-D-17-00105R2	Diffusing Diffusivity: A new derivation and comparison with simulations'	K. L. Sebastian	klsiisc@gmail.com	2-May

	L CHEMISTRY/ CHEMICAL DYNAMICS, July						
48	June	JCSC-D-17-00150R3	Synthesis, Characterization and Photoluminescence Properties of Tetra-amino Phenylporphyrin Covalently Linked to Multi-Walled Carbon Nanotubes'	R. Yamuna	ryamuna1@gmail.com	5-May	
49	June	JCSC-D-17-00138R1	Metal Free Synthesis of Functionalized 1-Aryl Isoquinolines via Iodine Mediated Oxidative Dehydrogenation and Ring Opening of Lactam in Isoindoloisoquinolinones'	Ramanathan C R	crrnath.che@pondiuni.edu.in;crram1@gmail.com	6-May	
50	June	JCSC-D-17-00147R2	Surfactant assisted sacrificial template mediated synthesis, characterization and photoluminescent properties of LaPO ₄ :Eu ³⁺ phosphor	Haq N Sheikh	hnsheikh@rediffmail.com	10-May	
51	June	JCSC-D-17-00209R1	SSZ-13 Supported Manganese Oxide Catalysts for the Low-Temperature Selective Catalytic Reduction of NO _x by NH ₃	Ruoyu Chen	cxdcry@163.com	10-May	
52	June	JCSC-D-16-01445R1	Can Uranyl Complexes Encapsulate to Carbon Nanotubes? A Periodic DFT Study'	Mahesh Sundararajan	smahesh@barc.gov.in	12-May	
53	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July	JCSC-D-17-00122R1	Facile Charge Transport in FeN _x /Mo ₂ N/CNTs nanocomposites for efficient hydrogen evolution reactions'	Ashok K Ganguli	ashok@chemistry.iitd.ac.in;ashokganguli@rediffmail.com	12-May	

54	June	JCSC-D-16-01189R1	olid-State Photodimerization in an Organic Salt of 1,2-Bis(4-pyridyl)ethylene and Trifluoromethanesulphonic Acid via Pedal-like Motion'	Abdul Malik Puthan Peedikakkal	abdulmalik@kfupm.edu.sa	14-May
55	June	JCSC-D-17-00012R1	Synthesis and cytotoxic evaluation of novel glycosylated N-fatty acyl tyrosine derivatives'	Ram Chandra Reddy Jala	jrcreddy10@gmail.com	14-May
56	August	JCSC-D-17-00240R2	Regioselectivity in the hetero-Diels-Alder reactions of styrenes with 2-aza-1,3-butadiene: A DFT study'	Safa Ali-Asgari	safa1308@yahoo.com	15-May
57	August	JCSC-D-17-00373	Low temperature synthesis of fluorite-type Ce based oxides of composition Ln ₂ Ce ₂ O ₇ (Ln = Pr, Nd and Eu): Photodegradation and luminescence studies'	Vithal Muga	mugavithal@gmail.com	18-May
58	August	JCSC-D-16-01284R2	Carboxylate Bridged Cu(II)coordination polymeric complex: Synthesis , Crystal structure, DNA binding, Magnetic Properties and electrochemical studies.'	Venkata Ramana Reddy Chittireddy	vrr9@yahoo.com	18-May
59	August	JCSC-D-17-00342R1	A Novel synthesis of chromone based unnatural α -amino acid derivatives	Manoranjan Behera	Manoranjan.Behera@gvkbio.com	
60	August	JCSC-D-16-01381R1	Phthalocyanine and azaphthalocyanines containing eugenol: synthesis, DNA interaction and comparison of lipase inhibition properties'	günay kaya kantar	gunay.kaya@erdogan.edu.tr	21-May
61	RAPID COMM August	JCSC-D-17-00371R1	Facile route for the regioselective synthesis of 1,4-disubstituted 1,2,3-triazole using copper nano particles supported on nano cellulose as recyclable heterogeneous catalyst	Diganta Sarma	dsarma22@gmail.com	21-May

62	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17- 00119R1	A Computational Investigation of the Red and Blue Shifts in Hydrogen Bonded Systems'	Swapan K Ghosh	skghosh@barc.gov.in	23-May
63	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		JCSC-D-17- 00180R1	On the Origin of Spurious Errors in Many-body Expansion for Water Cluster'	G N Sastry	gnsastry@gmail.com;gnsastry@iict.res.in	24-May
64	August		JCSC-D-17- 00363R1	Three coordination compounds based on benzene tetracarboxylate ligand: Syntheses, structures, thermal behaviors and luminescence properties'	Jun Qian	junqian8203@uj.edu.cn	29-May
65	August		JCSC-D-17- 00026R1	Synthesis, characterization and in vitro antibacterial activity of novel phthalazine sulfonamide derivatives'	<u>zahrasadat nazifi</u>	nazifi.zahrasadat@gmail.com	31-May
66	Special Issue - THEORETICAL CHEMISTRY/ CHEMICAL DYNAMICS, July		<u>JCSC-D-17- 00118R1</u>	Connecting Diffusion and Entropy for Water at the Single Particle Level	<u>Arnab Mukherjee</u>	arnab.mukherjee@iiserpune.ac.in	1-Jun
67	August		JCSC-D-17- 00295R1	Chaotropes trigger conformational rearrangements differently in Concanavalin A'	<u>Suman Jha</u>	jhas@nitrrkl.ac.in	1-Jun

68		JCSC-D-17-00389R2	Effect of Force and Location of Bottleneck for Particle Moving Through Window Under Encapsulation'	Pradip Kumar Ghorai	pradip.ghorai@gmail.com	4-Jun
69		JCSC-D-17-00410R1	Solvolysis of organophosphorus pesticide parathion with simple and α nucleophiles: a theoretical study'	Abhijit K Das	akdas64@gmail.com	4-Jun