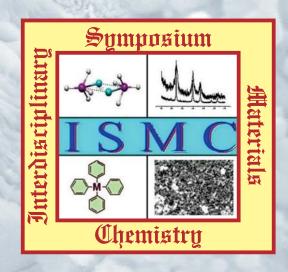
Proceedings of DAE - BRNS

8th Interdisciplinary Symposium on Materials Chemistry



June 17-19, 2021 Bhabha Atomic Research Centre Mumbai, India

Chemistry Division
Bhabha Atomic Research Centre
Trombay, Mumbai-400 085, India
&
Society for Materials Chemistry, India

Supported by
Board of Research in Nuclear Sciences
Department of Atomic Energy
Government of India





ISMC - 2020

Proceedings of DAE-BRNS 8th Interdisciplinary Symposium on Materials Chemistry

Bhabha Atomic Research Centre Mumbai, India

June 17 – 19, 2021

Organised by

Chemistry Division Bhabha Atomic Research Centre Trombay, Mumbai-400 085, India

&

Society for Materials Chemistry, India

Supported by

Board of Research in Nuclear Sciences
Department of Atomic Energy
Government of India

Proceedings of DAE-BRNS 8th Interdisciplinary Symposium on Materials Chemistry

Editors

Dr. Dimple Dutta

Dr. Pramod Sharma

Dr. ShilpaN. Sawant

Dr. K. C. Barick

Dr. Vinita G. Gupta

Dr. P. A. Hassan

June 2021 ISBN No. xx-xxxxx-xx-x

Printed, Designed and Processed by Chemistry Division
Bhabha Atomic Research Centre
Trombay, Mumbai-400085
E-mail: chemoff@barc.gov.in

Table of contents

M. S. no.	Title and Authors	Page no.
	Keynote Address	
	Catalytic Selectivity Engineering in Valorisation of Biomass, CO ₂ and Water into	1
	Chemicals, Materials and Energy	
	Prof. G. D. Yadav	
	Invited Talks	
IT-1	2D Metal Thiolates as Single Source Precursors for the Solvent Less Preparation of	3
	Semiconducting Metal and Bimetallic Sulfide Nanocrystals	
IT-2	Bhagavatula L. V. Prasad Pseudo 2-Dimensional Nanostructures: From Synthesis to Applications	5
11-2	D. Mandal, S. Biswas and Amreesh Chandra]
IT-3	Enhanced Atomic Ordering Leads to Ultra-High Thermoelectric Performance	7
	Kanishka Biswas	,
IT-4	Hot Carrier Relaxation in CsPbBr ₃ -Based Perovskites: A Polaron Perspective	8
	Hirendra N. Ghosh	
IT-5	Functionalized Supramolecular Assemblies: Platform for Unlimited Opportunities	9
TID 6	A. C. Bhasikuttan	1.0
IT-6	Development of Efficient Catalysts for Sustainable Chemical Industry	10
IT-7	M. Lakshmi Kantam Ionic Conductivity Pathways: A Neutron Diffraction Study	11
11-/	S. M. Yusuf	11
IT-8	Multiferroic Properties and Unconventional Spin Density Wave in Doubly Ordered	12
	PerovskiteNa <i>Ln</i> NiWO ₆ (<i>Ln</i> =Y, Dy, Ho, and Yb)	
	A. Sundaresan	
IT-9	Molecular Architectonics: De Nova Design of Advanced Functional Materials	13
	T. Govindaraju	
IT-10	Hybrid Metal-Ion Capacitors: Beyond Lithium	14
TT 11	M. M. Shaijumon	1.5
IT-11	Metal Organic Framework as a Nanosized Cavity to Stabilize the Protein Structure	15
	and Promote Catalytic Cctivity of Hybrid Myoglobin Abhijit Mondal, Mriganka Das and Shyamalava Mazumdar	
IT-12	Marvels of Nanotopography on Biomedical Implants	16
11 12	Deepthy Menon	10
IT-13	Soft-metamaterials: Synthesis and Characterization of Liquid Crystal-gold	17
	Nanoparticles	
	C. V. Yelamaggad	
IT-14	Electrochemical Sensors for Medical Diagnostic Application	18
	Shilpa N. Sawant	10
IT-15	Sensors for Monitoring Hydrogen in Sodium Systems	19
IT-16	E. Prabhu, N. Murugesan, Rajesh Ganesan and V. Jayaraman Establishing the Mechanism of Degradation of Ferritic/-Martensitic Steels in Lead Lithium	20
11-10	Eutectic to be used for Fusion Energy Applications	20
	Poulami Chakraboty, Raghvendra Tewari and Vivekanand Kain	
IT-17	Photofixation of Dinitrogen to Ammonia Under the Ambient Condition	22
	Kulamani Parida	
IT-18	Low-cost Materials for Cleaner Energy and Environmental Applications	24
	Nitin Labhasetwar	
IT-19	Elastic High Particle Content Nanocomposites by Ice-Templating	25
	Karthika Suresh, Sanat Kumar, Arindam Chowdhury, Soumyajyoti Chatterjee and Guruswamy Kumaraswamy	
	Short Lectures	
SL-1	Development of Functionalized Porous Materials andtheir Catalytic Applications	26
SL-I	Sk. Manirul Islam, P. Chakravorty, P. Sarkar, P.Mondal, M. Sarkar and M. Sengupta	20
SL-2	Effect of Dopant Oxidation States and O-vacancies in Catalysis	27
~2.2	K. Bhattacharyya	[
	~	

SL-3	SL-3 Development of Surface Engineered Nanomaterials for Cancer Theranostics K. C. Barick			
SL-4				
SL-5				
SL-6	Porous Material: A New Paradigm for Hydrogen storage Seemita Banerjee	31		
SL-7	Computational Modelling of Materials for Energy Applications Brindaban Modak			
	Nuclear Materials			
A-122	Effect of Elemental Distribution in the Laser Plume in Pulsed Laser Deposited Films meant for Mass Spectrometer Sampling U. K. Maity, P. Manoravi, M. Joseph and N. Sivaraman			
A-123	Response of Non-stoichiometric Pyrochlore Composition Nd _{1.8} Zr _{2.2} O _{7.1} to Electronic Excitations Saurabh Kumar Sharma, Vinita Grover, Rakesh Shukla, Abid Hussain and Pawan Kumar Kulriya	36		
A-124	Analysis of Diffusible Hydrogen in Modified 9Cr-1Mo Steel Weld by Gas Chromatography Technique Gopa Chakraborty, C. R. Das, M. Vasudevan and Shaju K. Albert	37		
A-125	Vaporisation Studies Over <ual<sub>2(cr)+U(cr)> Two Phase Region of U-Al System by using Knudsen Effusion Mass Spectrometry V.V. Trinadh, P. Manikandan, Suranjan Bera, C.V.S. Brahmananda Rao and T. S. Lakshmi Narasimhan</ual<sub>	38		
A-126	Sonochemically Exfoliation and Photodetection properties of Cu _{0.2} Sn _{0.8} Se Nanoparticles Kunjal Patel, Anand Patel and Vibhutiba P. Jethwa	40		
A-127	Neutron Diffraction Studies of Thorium Based Nuclear Fuel SourabhWajhal, Sonal Gupta, Raj Kumar, S. K. Satpati, A.B. Shinde and P.S.R. Krishna	41		
A-128	Corrosion Evaluation of Oxide Formed On Zircaloy-2 in Presence Of Metal Ions Sumathi Suresh and T.V. Krishnamohan	43		
A-129	Understanding the Materials Chemistry at Near Atomic Resolution Using Atom Probe Tomography Deodatta Shinde, Sudip Kumar Sarkar, Sanjay Saini, Amit Srivastava, Suman Neogy and Aniruddha Biswas	44		
A-130	Comparative Study on Durability of Thermal Insulations with High Temperature Sodium P.C. Clinsha, Jose Joseph, I. Lakshmigandhan, Raja Madhavan, R.Sudha, E. Senthilvadivu, K.H. Mahendran, K.I. Gnanasekar and V. Jayaraman	45		
A-131	Interplay of Grain Size and Irradiation Energy in the Radiation Response of Oxides Parswajit Kalita, Vinita Grover, R. Shukla, S. Ghosh, D. K. Avasthi and A. K. Tyagi	46		
A-132	Synthesis of Niobium Diboride by Carbothermic Reduction of Niobium Pentoxide D. S. Arati, T.S.R.C. Murthy, J. K. Sonber, Sanjib M. and A. K. Tyagi	48		
A-133	Preparation of U ₂ Ti Alloy by Direct Electrochemical Deoxidation Route L. Shakila, N. Sanil, R. Kumaresan and Kitheri Joseph	49		
A-134	Trace Elemental Analysis using Total Reflection X-Ray Fluorescence Spectroscopy S. Dhanavel, R. Raja Madhavan and R. Asuvathraman	50		
A-135				
A-136				
A-137	Investigation of Inhomogeneity in Metal Alloys using Laser Induced break down Spectroscopy J. Namitha, M. Rahaman, U. K. Maity, P. Manoravi, S. Das, M. Joseph and N. Sivaraman	56		
A-138	Thermochemical Properties of T-91clad Using Knudsen Effusion Mass Spectrometry V.V. Trinadh, P. Manikandan, Suranjan Bera, C.V.S. Brahmananda Rao and T. S. Lakshmi	58		

A-139	A Novel and Greener Approach of External (in air) PIGE at FOTIA Towards	59
	Preparation of <i>In House</i> Reference Materials of Boron Carbides for Isotopic	
	Composition of Boron	
	Sk Wasim Raja, R. Acharya and P. K. Pujari	
A-140	Anion (131) Diffusionin Altered Fe-montmorillonite Clay Minerals Relevant to	61
	Geological Waste Disposal	
	Santosh Chikkamath, Madhuri A Patel, Aishwarya S Kar, Sumit Kumar, Tomar B.S. and	
A 1.41	Jayappa Manjanna Determination of Solvhility Limit of CaE, in IMSDD Coolant Solt ELiNoV	63
A-141	Determination of Solubility Limit of CrF ₂ in IMSBR Coolant Salt FLiNaK	03
A-143	Rimpi Dawar, S. Kolay and R. Mishra Quality Assurance during the Non-destructive EDXRF Determination of Nb in Zr-Nb	65
A-143	Alloy	03
	Remya Devi P.S, Trupti A. Chavan and K.K. Swain	
A-143	High-Pressure High-Temperature Structural Stability of Zeolite-A	66
	K. A. Irshad, N. R Sanjay Kumar, M. Mahima Kumar and Hrudananda Jena	
A-144	A Novel Ligand for Selective Precipitation of Uranyl Ion with Fast Kinetics	67
	Bal Govind Vats, Kaushik Sanyal, Mukesh Kumar and S. Kannan	
A-145	Thermal Degradation Studies of Paint Used in Indian Nuclear Containment Building	68
	Subhamoy Saha, Ajit N. Shirsat, V. S. Tripathi, Salil Varma and P. Mathi	
A-146	Compatibility of Ni-Mo-Cr Alloys with Fluoride Salt at Elevated Temperature	69
	Rumu H. Banerjee, P. Chakraborty, Vishal Singh, Vijay Karki and R. Tewari	
A-147	Role of Clay Microstructure in Caesium Diffusion through Compacted Bentonite	71
	Annapurna Chandane, Arijit Sengupta, V. B. Jayakrishnan, P. U. Sastry, R. K. Bajpai, and	
1 1 10	Sumit Kumar	70
A-148	Thermodynamic Properties of 3C Silicon Carbide-an <i>ab initio</i> investigation	72
A-149	Razmi Das, Ananth S Iyengar, Mala N Rao, Devesh Raj and R S Keshavamurthy Development of High Entropy Alloys For Advanced Nuclear Reactors	73
A-149	P. Chakraborty, C. Patil, N. K. Sarkar, B. Vishwanadh, J. Jha, G. Sugilal, R. Tewari and S.	13
	Banerjee	
A-150	Preparation and Characterization of Iron-Zirconium Binary Alloys	74
11 100	Sourav Majumder, Dheeraj Jain and V. Sudarsan	, .
A-151	Characterization of Residue Ash from Plasma Incineration of Simulated Radioactive	75
	Waste	
	Keyur Pancholi, Param Jeet Singh, Anita Gupta, S. R.Vishwakarma, D. V. Udupa and C. P.	
	Kaushik	
A-152	Neutron Emission Characterisation with Silver Activation Counters at Dense Plasma	77
	Focus Device	
	J.Balu Naik, Rishi Verma, S K Sharma, J N Rao, B.K Das, M. Meena, Lakshman R and	
A 152	A Study on TI Duild up in The Broduct Student of Bornesseeing Facility	70
A-153	A Study on Tl Build-up in The Product Stream of Reprocessing Facility P. K. Sharma, Piyali Banerjee, T. P. Valsala, D. B. Sathe and R. B. Bhatt	78
A-154	Lattice Thermal Expansion of ScPO ₄ and ScVO ₄	79
A-134	Sneha Suresh, S. J. Patwe, S. N. Achary and A. K. Tyagi	1)
A-155	Direct Preparation of U-7Nb Alloy from (U,Nb)mixed oxides	80
A-133	Mohd. Sufiyan Khan, Anwesha Mukherjee, R. Kumaresan, and Kitheri Joseph	00
A-156	Effect of Synthesis Route on Desintering in Nanocrystalline Thoria	82
11 100	Dheeraj Jain, V. Sudarsan and A. K. Tyagi	
A-157	Formation and Stability of Pyrochlore Type CaCeTi ₂ O ₇	83
	Shrikant Padhy, Rakesh Shukla, A. K. Sahu, S. N. Achary and A. K. Tyagi	
A-158	Phase stability and phase transformation in $U-(6-x)Zr-xNb$ alloys (x = 0, 2, 4, 6 wt%)	84
	Santu Kaity, Joydipta Banerjee, S.C. Parida and P.G. Behere	
A-159	Development of Plasma Spray Coating of Yttrium Phosphate on Molybdenum	85
	Substrate for Containment of Molten Metals	
	S. Bhandari, N. Tiwari, Y. Chakravarthy, V. Chaturvedi Misra, S Ghorui and T. Mahata	
A-160	Radiation Induced Changes in Microbial characteristics of Spices using 10MeV	86
	Electron Beam Accelerator	
	Sirisha Majji, Vanshika Adiani , A.S. Dhavale and Archana Sharma	

		0.5
A-161	Investigation of Phase Equilibria in SrO-La ₂ O ₃ -P ₂ O ₅ System Geeta Patkare, Meera Keskar, and S. Kannan	87
A-162	Thermo-physical Properties of Strontioum Lanthanum Phosphates	88
A-102	Geeta Patkare, Muhammed Shafeeq, Meera Keskar, R.A. Phatak and S. Kannan	00
A-163	Synthesis and Characterization of Simulated Corrosion Products for Optimisation of	89
	Decontamination Processin Boiling Water Reactors	
	V. Balaji, P. Chandramohan, Puspalata Rajesh and T.V. Krishna Mohan	
	Nanomaterials	
B-121	Copper Immobilized Polyaniline/Multiwalled Carbon Nanotube Nanocomposites for	90
	Catalytic and Antibacterial Properties	
	S. P. Deshmukh, D. K Dalavi and S. D. Delekar	
B-122	Dual Mode Behaviour of Ho ³⁺ , Yb ³⁺ and K ⁺ co-doped YVO ₄ Nanophosphor for its	91
	Optical and Hyperthermia Applications	
	Ramaswamy S. Perala, B. P. Singh, P.V. Nagendra Kumar, R. Acharya and R.S. Ningthoujam	
B-125	RGB Emission and Solar Efficiency Enhancement in Eu ³⁺ , Tb ³⁺ Activated/co-	92
	activated K ₂ NaAlF ₆ Downconversion Phosphors by Energy Transfer Mechanism	
	Abhijeet R. Kadam and S. J. Dhoble	
B-126	Synthesis, Characterization and Biological Applications of Pure and Bio - modified	93
	TiO ₂ Nanoparticles	
	P. Maheswari , S.Ponnusamy, S. Harish , M. Navaneethan , K. D. Nisha, Ganesh Munuswamy	
D 127	Ramanujam and Y. Hayakawa	0.4
B-127	Hypoxia Responsive Nanoparticle Conjugates for Anticancer Drug Delivery	94
	Rashmi Kumari, Vasumathy R, Dhanya Sunil, Raghumani Singh Ningthoujam, Srinivas Mutalik and Badri Narain Pandey	
B-128	Influence of Laser Polarization on Dynamics of Gas-Phase Nanoclusters: A Case	95
D-120	Study on (CCl ₄) _n Clusters)3
	P. Sharma and S. Das	
B-129	Structural and Solid-State Properties of Mn Substituted Ni-Zn Ferrites Synthesized by	96
2 12	Combustion Method	
	Seneca O. Costa and V.M.S. Verenkar	
B-130	Biogenic synthesis of ZnO nanoparticles using <i>Annonamuricata</i> plant leaf extract and	98
	its anti-cancer efficacy on 2D and 3D tumor models	
	Siva Chander Chabattula, Piyush Kumar Gupta, Rama Shanker Verma, Debashis Chakraborty	
B-131	Combustion Triggered Route for Synthesizing Nanostructured Nickel Substituted	99
	Cobalt Ferrites: Investigations on their Structural, Morphological, Electrical,	
	Dielectric and Magnetic Properties	
	Mangala U. Sawal and V. M. S. Verenkar	
B-132	Study of Interaction of a Coagulating Agent Protamine Sulfate with Lipid Bio-	100
	Membrane	
D 122	Ripa Paul, Surajit Sarkar, Hritinava Banik, Debajyoti Bhattacharjee, Syed Arshad Hussain	101
B-133	Comparative Studies of Electrical Properties of Tin Doped BaTiO ₃ Synthesized Via	101
	Two Different Low Temperature Routes Richa Tomar, Karan Surana, Pankaj Gupta and N. B. Singh	
B-134	X-Ray Diffraction Analysis of Hexagonal Klockmannitecuse Nanoparticles and its	102
D-134	UV Photodetection Property	102
	Kunjal Patel, Anand Patel and Vibhutiba P. Jethwa	
B-135	Polymeric Scaffold of Gallic Acid Loaded Chitosan Nanoparticles Infused With	103
D 100	Collagen-Fibrin for Wound Dressing Application	100
	Pallavi Shyam Kaparekar , Srinivetha Pathmanapan ^a and Suresh Kumar Anandasadagopan	
B-136	Cyclic Voltammetry Performance of La-doped SrTiO ₃ Electrodes for Supercapacitor	104
	Applications	
	V. V. Deshmukh, H. P. Nagaswarupa, C. R. Ravikumar, and N. Raghvendra	
B-137	Tailoring Electronic and Optical Properties of Graphene Quantum Dots by	105
	Heteroatom Nitrogen Doping	
	Tushima Basak and Tista Basak	
B-138	Use of Single Source Precursor for the Synthesis of Wurtzite Form of Zns	106
	Nisha Kushwah, A. Wadawale, G. Kedarnath, V. Sudarsan and R. M. Kadam	

Structural and Solid-State Properties of Mn Substituted Ni-Zn Ferrites Synthesized by Combustion Method

Seneca O. Costa and V.M.S. Verenkar*

School of Chemical Sciences, Goa University, Taleigao Plateau, Goa 403206, India

* E-mail: vmsv@unigoa.ac.in; Contact no.: +91-9822980123

Malic acid which is a dicarboxylic acid can act as an excellent fuel due to its low ignition temperature, high calorific value, non-explosive and low cost. To improvise the basic properties of Ni-Zn ferrites for example, to attain magnetic properties with low losses especially at high frequencies, etc., we decided to synthesizeMn substituted Ni-Zn ferrites using Malic acid as the fuel via combustion route.

A novel series of nano-sized $Zn_{0.5-x}Mn_xNi_{0.5}Fe_2O_4$ (x= 0.1-0.3) were prepared using metal nitrates and Malic acid as fuel in the ratio of 1:0.97 by combustion technique after optimization.

XRD studies confirmed the formation of single-phase cubic spinel ferrites [1]. The crystallite size ranged between 10-23 nm. The IR spectra showed the presence of two M-O stretching vibrations in the frequency range of 800-350 cm⁻¹ which are the characteristic bands of spinel ferrites. EDX spectra confirmed the presence of desired elements and SEM image showed spherical particles with agglomeration. A decrease in resistivity was observed with rise in temperature indicating the semiconducting behaviour of spinel ferrites [2]. Also fall in resistivity was seen with increase in Mn content. Curie temperature was seen increasing with increase in Mn concentration. Normal behaviour of spinel ferrites was observed in dielectric studies where a sharp decrease in dielectric constant at lower frequencies was observed which remains constant with further increase in frequency [3]. Relaxation peaks for all the synthesized ferrites were observed which occur when the hopping frequency is equal to the externally applied frequency [4].

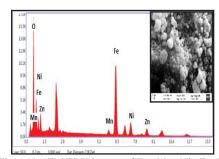


Figure 1. SEM/EDX images of Zn_{0.4}Mn_{0.1}Ni_{0.5}Fe₂O₄

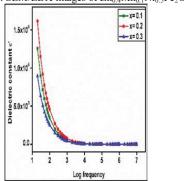
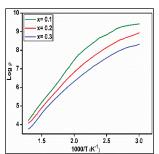


Figure 3. Plot of dielectric constant v/s frequency



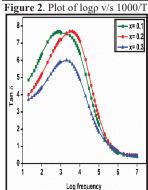


Figure 4. Plot of tan δ v/s frequency

 $\textbf{Table 1:} \ Crystallite \ size \ (D), M-O_{tetra} \ (\upsilon_1) \ and \ M-O_{oct}(\upsilon_2) stretching \ vibrations \ in \ IR \ spectra \ and \ Curie$

temperature (Tc)

X	D nm	υ ₁ (cm ⁻¹)	υ ₂ (cm ⁻¹)	Tc (K)	
0.1	22.81	592	409	633	
0.2	18.47	597	408	678	
0.3	10.35	598	408	708	

A novel series of $Zn_{0.5-x}Mn_xNi_{0.5}Fe_2O_4$ (x= 0.1-0.3) spinel nano-ferrites were synthesized by combustion method. The 'as prepared' ferrites were characterized by XRD, IR, SEM/EDX and AC susceptibility. Electrical resistivity measurements confirmed the semiconducting nature of Mn substituted Ni-Zn ferrites. Dielectric properties were studied as a function of frequency which showed a normal behaviour of spinel ferrites.

References:

- 1. T.S. Kuru, M. Kuru and S.Bağcı, J. Mater. Sci.: Mater. Electron., 29 (2018) 17160-17169.
- 2. A.A. Sattar, H.M. El-Sayed, K.M. El-Shokrofy and M.M. El-Tabey, J. Mater. Sci., 42 (2007) 149-155.
- 3. A. Amarendra, K. Singh, T.C. Goel, R.G. Mendiratta, O.P. Thakur and C. Prakash, *J. Appl. Phys.*, 91 (2002) 6626.
- 4. S. Ramesh, B. Dhanalakshmi, B.C. Sekhar, P.S.V.S. Rao and B.P. Rao, Ceram. Int., 42 (2016)9591–9598.