DR. VENKATESWARARAO ALAPARTHI

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K.L University *venkateswararao.alaparthi@gmail.com*
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CAREER OBJECTIVE:

To take up the challenging tasks and strive for excellence of the organization with my strong determination and loyalty.

EDUCATIONAL PROFILE:

- **Ph.D (F.T)** in the field of Materials Science (on solid electrolytes for Li-ion Batteries in May-2013) from Department of Physics under the guidance of **Prof. V.Veeraiah**, Andhra University, Visakhapatnam, Andhra Pradesh.
  Thesis title: *Synthesis and characterization of* Fe^{3+}, Mn^{4+}, Zr^{4+}, Sn^{4+} *and* V^{5+} *doped* $LiTi_2(PO_4)_3$ *materials as electrolytes for Lithium-ion batteries.*

- **M. Sc** (Physics) with **73.40%** Acharya Nagarjuna University in the year 2007 from N.R.K & K.S.R Gupta Degree College, Tenali, Guntur District, Andhra Pradesh.

- **B. Sc** (MPG) with **63.11%,** Acharya Nagarjuna University in the year 2000-03 from V.S.R & N.V.R Degree College, Tenali. Guntur District, Andhra Pradesh.

- **XII** (CBSE) with **65%** in the year 2000 from Jawahar Navodaya Vidyalaya, Maddirala, Guntur District, Andhra Pradesh.

- **X** (CBSE) with **72.20%** in the year 1998 from Jawahar Navodaya Vidyalaya, Maddirala, Guntur District, Andhra Pradesh.

TECHNICAL QUALIFICATIONS:

- Microsoft Office, internet

TEACHING EXPERIENCE:

- Working as Assistant Professor in **Department of Physics, K. L. University,** Vaddeswaram, Guntur District, Andhra Pradesh since July-15, 2013.

RESEARCH EXPERIENCE:

- Published papers in 6 International journals, 2 National journals.
- Reviewer for International journal of **Science and Engineering of Composite Materials**
- Mentor for four (5) part-time Ph. D scholars.

PROJECTS:

- **Principle Investigator** for **DST-SERB, Young Scientist** project worth 37.54 Lakhs, file number: **SB/FTP/ETA-0176/2014 (2015-2018).**
- **Title:** Synthesis, characterization and evaluation of nano structured spinel thin-film $LiMn_2O_4$ cathode active materials with hetero valent multi ion insertion: Application for rechargeable micro batteries.

CHARACTERISTICS & SKILLS:

- Have good desire to work hard and learn more there by updating the knowledge with the changes. Dedication and determination to perform
- Open mind to explore new horizons
- Positive attitude, self confidence and belief in hard work

PERSONAL PROFILE:

Name	:	**VENKATESWARARAO ALAPARTHI**
Father's Name	:	Sri A. Chittiah
Date of Birth	:	10-06-1982
Gender	:	Male
Nationality	:	Indian
Religion	:	Hindu
Hobbies	:	Reading Books
Languages Known	:	English, Hindi & Telugu
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DECLARATION:

I am also confident to my ability to work in a team. I hereby declare that the above statements are true to the best of my knowledge.

Place **:** Vaddeswaram

Date **:** (A. VENKATESWARA RAO)

REFERENCES:

1 ***Prof. V.Veeraiah***
Department of Physics (at present Vice-Chancellor of Vikrama Simhapuri University, Nellore, A.P)
Andhra University
Visakhapatnam-03

2 ***Prof. A.V. Prasada Rao (Retired)***
Department of Inorganic and Analytical Chemistry
Andhra University
Visakhapatnam-03

3 ***Dr. B. Kishore Babu***
Assistant Professor
Department of Engineering Chemistry
Andhra University
Visakhapatnam-03

NATIONAL CONFERENCES:

1. **A.Venkateswara Rao**, V.Veeraiah, B.Swarna Latha National Seminar on *Recent Advances in Physics-2011,* Recent Advances in Physics" held during 5-6 January 2011 *at P. R. Govt. College, Kakinada, A.P., India, "Structural and impedance spectroscopic study of* $LiTi_2(PO_4)_3$*".*
2. **A.Venkateswara Rao**, V.Veeraiah, B.Swarna Latha, national conference on "Advanced Research Concepts in Physics" held during 24th & 25th of November 2011 at Government College, Rajahmundry, Andhra Pradesh, India, "*Synthesis and Study of ceramic Lithium Titanium Phosphate".*
3. **A.Venkateswara Rao**, V.Veeraiah, B.Swarna Latha, National Seminar on *Recent Trends in Advanced materials-2012,* held during 27th & 28th of January 2012 at Sir C.R. Ready (A) College, Eluru-534007, Andhra Pradesh., India *"Structural and Vibrational spectroscopic study of* $LiTi_2(PO_4)_3$*".*
4. **A.Venkateswara Rao**, V.Veeraiah, B.Swarna Latha National Seminar on *Recent Advances in Applied Chemistry-2011.*
5. B. Swarnalatha, **A.Venkateswara Rao**, V.Veeraiah, V. Raviraju, B.Kishore Babu, National Seminar on *Recent Trends in Advanced materials-2012,* held during 27th & 28th of January 2012 at Sir C.R. Ready (A) College, Eluru-534007, Andhra Pradesh., India *"Recent advances in lithium ion technology".*
6. B. Swarnalatha, **A.Venkateswara Rao**, V.Veeraiah, V. Raviraju, B.Kishore Babu, National seminar on "*Recent advances of Spectroscopy in chemistry*" 27th Febraury, 2012. "*Recent advances in Nano sized lithium ion batteries*".
7. B. Swarnalatha, **A.Venkateswara Rao**, V.Veeraiah, V. Raviraju, B.Kishore Babu, National conference on "*chemistry for sustainable development*" *(suscon-2012)*

October 10-11, 2012, A new Lithium Titanium Phosphate materials for power source cells and their physiochemical properties.

8. K. Ephraim Babu, N. Murali, K. Vijay Babu, **A.Venkateswara Rao**, K. Rama Rao, V.Veeraiah, National Seminar on *Computational Techniques for Engineering Applications (NSCTEA-2012) Nov 9-10,2012.* Computational Study of Structural, Electronic and Optical Properties of Cubic $BiInO_3$, Corporate Institute of Science and Tech., Bhopal (M.P).
9. N. Murali, K. Ephraim Babu, K. Vijay Babu, **A.Venkateswara Rao**, K. Rama Rao, N. Gnana Praveena, A. Mary Vijay Ratna and V.Veeraiah. *National conference on Green Energy & Sustainable Methods (GESM-2012),* Density Functional theoretical study of structural, electrical and optical properties of cubic perovskite semiconductor $BiAlO_3$. M.R College-Vizianagaram, Nov 9th &10th 2012.
10. K. Ephraim Babu, N. Murali, K. Vijay Babu, **A.Venkateswara Rao**, K. Rama Rao, N. Gnana Praveena, A. Mary Vijay Ratna and V.Veeraiah. *National conference on Green Energy & Sustainable Methods (GESM-2012),* First principal Study on the Structural, Electronic and Optical Properties of Cubic perovskite $BiGaO_3$. M.R College-Vizianagaram, Nov 9th &10th 2012.
11. Participated in National workshop on Global Warming on Water Quality [GWIW-2013] in the department of Engineering Chemistry, Andhra University, Visakhapatnam on 22nd March, 2013.
12. Participated in the workshop on 'Recent Trends in Fuel cell Technologies' held on 26th Sep, 2014 at centre for Advanced Energy Studies (CAES), K L University.
13. Participated in two day National workshop on “Emerging Trends in Renewable Energy (NWETR-2015” organized by Electrical and Electronics Engineering and Centre for Advanced Energy studies at K L University on 18th and 19th March, 2015.
14. Participated in 7th National symposium for materials research scholars, IIT Bombay from 20-22 May, 2015 with title “Nano Scale Solid Electrolyte for Lithium-Ion Batteries”.

INTERNATIONAL CONFERENCES:

1. Paper presented in “International Conference of Young Researchers on Advanced Materials” at Biopolis, Singapore, July 1-6, 2012 on “*Recent Advances in Li-ion batteries*” by B.Swarna LATHA, B. kishore BABU, **VenkateswaraRao ALAPARTHI**, veeraiah VALAPARLA.

2. Paper presented in “International symposium on Effluents and Emissions on Environment and Energy” at Department of Engineering Chemistry, A.U College of Engineering, Andhra University, Visakhapatnam, Dec 23-24, 2011 by B.Swarna LATHA, V. Raju, **VenkateswaraRao ALAPARTHI**, B.kishore BABU, veeraiah VALAPARLA.

PUBLICATIONS:

1. **Effect of Mn substitution on the electrochemical properties of $LiTi_2(PO_4)_3$**

   A.Venkateswara Rao[*a], V.Veeraiah[a], A.V.Prasada Rao[b], B.Kishore Babu[c]

   [a]Department of Physics, [b]Department of Inorganic and Analytical Chemistry, [c] Department of Engineering Chemistry; Andhra University, Visakhapatnam-India

   Chem Sci Trans., 2013, 2(1), 105-112 (Chemical Science Transactions)

2. **Effect of Fe^{3+} doping on the structure and conductivity of $LiTi_2(PO_4)_3$**

   A.Venkateswara Rao[*a], V.Veeraiah[a], A.V.Prasada Rao[b], B.Kishore Babu[c]

   [a]Department of Physics, [b]Department of Inorganic and Analytical Chemistry, [c] Department of Engineering Chemistry; Andhra University, Visakhapatnam-India

   Res Chem Intermed 41 (2015) 2307–2315 ***(IF 1.883)***

3. **Structural, Spectroscopic and Electrochemical Study of V^{5+} Substituted $LiTi_2(PO_4)_3$ Solid Electrolyte for Lithium-ion Batteries**

   A.Venkateswara Rao[*a], V.Veeraiah[a], A.V.Prasada Rao[b], B.Kishore Babu[c], B.Swarna Latha[a], K.Rama Rao[a]

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   Bull. Mater. Sci, Vol. 37, No. 4, June 2014, pp. 883–888 ***(IF 0.895)***

4. **Spectroscopic characterization and conductivity of Sn substituted $LiTi_2(PO_4)_3$**

   A.Venkateswara Rao[*a], V.Veeraiah[a], A.V.Prasada Rao[b], B.Kishore Babu[c] **,** M.Brahmayya[c]

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   Res Chem Intermed (2015) 41:4327–4337 ***(IF 1.883)***

5. **Influence of Zr^{4+} doping on structural, spectroscopic and conductivity studies of Lithium Titanium Phosphate,** **A.Venkateswara Rao**[*a], V.Veeraiah[a], A.V.Prasada Rao[b], B.Kishore Babu[c] **,** K.Vijaya Kumar[a]

   [a]Department of Physics K.L.University, Vaddeswaram; [b]Department of Inorganic and Analytical Chemistry, [c] Department of Engineering Chemistry; Andhra University, Visakhapatnam-India

   Ceramics International 40 (2014) 13911– 13916 ***(IF 2.758)***

6. **Atomic-Scale Finite Element of Post Buckling CNT'S,** V.PRASANTHI[a], K. SUNIL BABU[b], **A.VENKATESWARA RAO**[c],

   [a] Department of Physics, JNTUK, VZM Campus, [b] Department of Physics Miracle Engg. College Bhogapuram, A.P, [c] Department of Physics, K L University, Vaddeswaram, Guntur, India

   International Journal of Innovative Technology and Research 2,4 (2014) 1151 – 1156 .

7 **Synthesis, characterization and phase transition studiesin 4-hexyloxy benzylidene 4’-alkoxyanilines**
K. Sunil Babu[a], A. Venkateswara Rao[a], P. V. V. Kishore[b], P. Pardhasaradhi [b],
B. T. P. Madhav [b] and V. G. K. M. Pisipati
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PHASE TRANSITIONS, 2016, 1-12. ***IF 0.8585***

8 **Estimation of thermodynamic parameters in 4-(hexyloxybenzylidene)-4′alkoxy anilines, 6O·Om liquid crystalline compounds – A density study**
K. Sunil Babu [a], A. Venkateswara Rao [b], D. Madhavi Latha [c], P. Pardhasaradhi [d], V.G.K.M. Pisipati [d],
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Journal of Molecular Liquids 220 (2016) 999–1003. ***IF 2.740***

9 **Estimation of orientational order parameter from different models in 6O·Om LC materials - an optical study**
K. SUNIL BABU[1], A. VENKATESWARA RAO[1], B. T. P. MADHAV[2],P. V. V. KISHORE[2], P. PARDHASARADHI[2] and V. G. K. M. PISIPATI[2]
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International Journal of Modern Physics: Advances in Theory and Applications

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RESEARCH ARTICLE

Effect of Mn Substitution on the Electrochemical Properties of $LiTi_2(PO_4)_3$

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Received 21 July 2012 / Accepted 16 August 2012

Abstract: Mn substituted $LiTi_2(PO_4)_3$ samples of composition $LiMn_xTi_{2-x}(PO_4)_3$ (x=0.0, 0.1, 0.3 and 0.5) have been prepared by solid-state method. XRD studies indicated formation of phase pure materials of rhombohedral structure. Micro structural studies by scanning electron microscopy (SEM) revealed particle size in the range of microns. Conductivity results from 313 K to 573 K showed high ionic conductivity for low amount of Mn and electronic conductivity results are well correlated with ionic conductivity studies. Cyclic voltammetry results showed its electrochemical stability and reaction mechanism in the voltage range from 0.5 to 3.5 V.

Keywords: Lithium titanium phosphate, Mn doped $LiTi_2(PO_4)_3$, Ionic conductivity, Electronic conductivity

Introduction

Exploitation of insertion oxides as host materials for rechargeable batteries has been the subject of many researchers to power several portable electronic devices such as cell phones, laptops, digital cameras *etc.* Since no other cations except H^+ can penetrate easily into solids than Li^+, the study of rechargeable Li batteries has been actively pursued since 1970s with lithium insertion electrodes in the form of layered $LiCoO_2$ and spinel type $LiMn_2O_4$[1-3]. Besides these two host materials, complex phosphates like $LiTi_2(PO_4)_3$ (LTP) with NASICON [$Na_3Zr_2(SiO_4)_2(PO_4)$] structure have also been explored because of their high ionic conductivity, low thermal expansion coefficient, and low thermal conductivity[4]. In view of competitive energy-density storage and better thermal properties, phosphate based materials are potential candidates as cathodes for lithium ion batteries compared to traditional cathodes like $LiCoO_2$, $LiMn_2O_4$, V_2O_5, *etc*. LTP structure is made up of two TiO_6 octahedra linked with three PO_4 tetrahedra via oxygen sharing. Lithium is present in two different types of interstitials formed by six oxygen atoms and eight oxygen atoms respectively. These two interstitials arranged alternatively along the conduction channels provide a three dimensional network for Li-ion transport[5]. The conductivity of these materials

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Effect of Fe^{3+} doping on the structure and conductivity of $LiTi_2(PO_4)_3$

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A. V. Prasada Rao · B. Kishore Babu

Received: 4 April 2013 / Accepted: 19 July 2013 / Published online: 7 August 2013

Abstract Fe^{3+}-substituted $LiTi_2(PO_4)_3$ samples of composition $Li_{1+x}Ti_{2-x}Fe_x(PO_4)_3$ ($x = 0.0, 0.05, 0.1$, and 0.15) have been prepared by solid-state reaction. XRD studies indicated formation of phase-pure materials of rhombohedral structure. Microstructural studies by scanning electron microscopy revealed particle size was in the micron range. Conductivity data at 533 and 573 K revealed increasing ionic conductivity with increasing dopant concentration. Electronic conductivity results correlated well with ionic conductivity. Cyclic voltammetry studies were indicative of electrochemical stability in the voltage range 0.5 to 3.5 V.

Keywords Lithium titanium phosphate · Nasicon material · Fe-doped $LiTi_2 (PO_4)_3$ · Ionic conductivity · Electronic conductivity · Cyclic voltammetry

Introduction

Nasicon (sodium super ionic conductors) structured lithium titanium phosphate (LTP) ceramics have been studied as promising solid electrolytes for lithium batteries [1, 2]. LTP structure is made up of two TiO_6 octahedra linked with three PO_4 tetrahedra via oxygen sharing. Lithium is present in two different types of

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Res Chem Intermed (2015) 41:4327–4337
DOI 10.1007/s11164-014-1532-x

Spectroscopic characterization and conductivity of Sn-substituted $LiTi_2(PO_4)_3$

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A. V. Prasada Rao · B. Kishore Babu · M. Brahmayya

Received: 17 October 2013 / Accepted: 3 January 2014 / Published online: 18 January 2014

Abstract Sn-doped $LiTi_2(PO_4)_3$ samples of composition $Li[Ti_{2-x}Sn_x](PO_4)_3$ ($x = 0$–0.5) are prepared by solid-state reaction. XRD results are indicative of formation of phase-pure materials of rhombohedral structure with the space group $R\bar{3}c$ (167). Study of the microstructure by scanning electron microscopy (SEM) revealed particle size was in the range 0.6–1 μm and that grain size decreased with increasing Sn content. Raman spectra contained peaks at high frequencies ascribed to intramolecular PO_4^{3-} stretching modes. Study of electrochemical impedance up to 573 K revealed high ionic conductivity of 2.02×10^{-4} S/cm at room temperature for $x = 0.1$.

Keywords Nasicon materials · X-ray diffraction · Lithium titanium phosphate · Sn doped $LiTi_2(PO_4)_3$

Introduction

Because of their structure, sodium superionic conductors (Nasicon) have interesting properties when substituted with trivalent and tetravalent cations. These materials are important improved solid electrolytes because of their three-dimensional framework structure with high ionic conductivity comparable with that of two-dimensional networks, for example β-alumina [1]. $LiTi_2(PO_4)_3$ (LTP) has the

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CERAMICS INTERNATIONAL

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Influence of Zr^{4+} doping on structural, spectroscopic and conductivity studies of lithium titanium phosphate

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Abstract

Zirconium doped $LiTi_2(PO_4)_3$ (LTP) samples with the chemical composition of $Li[Ti_{2-x}Zr_x](PO_4)_3$ (x=0.0, 0.1, 0.3 and 0.5) are prepared by solid state reaction method. XRD data revealed the formation of phase pure materials of rhombohedral structure with space group $R\overline{3}\ c$(#167). Microstructural studies by scanning electron microscopy indicated that the particle size is in the range of 0.5–1 μm. Raman spectroscopic study showed that the peaks at high frequencies are due to intramolecular PO_4^{3-} stretching modes. Electrochemical impedance studies showed high ionic conductivity for small amount of Zirconium (x=0.1) doping.

Keywords: X-Ray diffraction; Nasicon materials; Lithium titanium phosphate; Zirconium doped $LiTi_2\ (PO_4)_3$

1. Introduction

Nasicon (Sodium Super Ionic Conductors) compounds of rhombohedral symmetry with (space group $R\ \overline{3}\ c$) find potential applications as electrolytes for lithium-ion batteries [1,2]. These ionic conductors display a three dimensional conducting network where superionic conductivity may occur [3,4]. The original NASICON materials are synthesized with general formula $Na_{1+x}Zr_2P_{3-x}Si_xO_{12}$ $(0 \leq x \leq 3)$. After the synthesis of NASICON materials, a large number of phosphate related materials are synthesized by partial substitution of tetravalent cations by trivalent [5], tetravalent [6] and pentavalent cations [7,8]. Since Li has unmatchable properties with high potential (E^0=23.024 V), the research on Li based LISICON solid electrolytes has become the prominent subject for all solid lithium batteries.

In the structure of LISICON materials $A_xB_y(PO_4)_3$, PO_4 tetrahedra are linked by the corners to MO_6 octahedra. The infinite ribbons resulting from this linkage are connected together, perpendicular to the *c* direction, by PO_4 tetrahedra to form the framework. The Li^+ ions occupy two positions in the conduction channels: the M1 site (one per formula) is coordinated by a trigonal antiprism of oxygens, and the M2 site (three per formula) has a distorted 8-fold coordination. M1 and M2 sites are located inside and between the ribbons, respectively [9,10]. The effect of Zr substitution in Ti^{4+} site showed some observable changes in the structure and phase [1,11].

In the present work, the $LiTi_{2-x}Zr_x(PO_4)_3$ series $(0.1 \leq x \leq 0.5)$ of samples have been prepared and studied by XRD, SEM, RAMAN spectra and Electrochemical Impedance spectroscopy techniques. Structural changes and phase identification are explained by XRD. Morphology of materials is investigated by

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Research Article

Atomic-Scale Finite Element of Post Buckling CNT'S

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Abstract: - **This paper illustrates an atomic-scale finite element method AFEM to study the post buckling behavior of Carbon Nano Tubes CNTs. The computed energy curves and critical strain for the (8, 0) single-walled CNT SWNT agree with atomistic simulations. The AFEM is very fast and flexible outstanding to the competence of the finite element method. For the SWNT, the strain energy curves have apparent jumps at morphology changes and during the smooth continuation stages of post buckling, the strain energy varies in the linear order with the strain. For the double-walled CNT, there are only small strain energy releases, and the strain energy also changes approximately piecewise linearly with the strain. The morphologies are obtained in detail. AFEM is computationally rapid and is an alternative efficient way to study the post buckling of CNTs.**

Keywords: - **Atomic-Scale Finite Element Method; Post Buckling; Carbon Nano Tube (CNT)**

I. INTRODUCTION

Experimental analysis and hypothetical research have displayed exclusive mechanical properties of carbon nanotubes CNTs[1-2]. Large deformation of CNTs in the post buckling stage was found in the atomic force microscope test of Falvo[5] and the transmission electron microscopy test of Lou-rie[6]. Because there are few quantitative investigational results on their post buckling characteristics, extensive hypothetical research has been carried out to examine their post-buckling behavior. In general, the widely used theoretical methods include atomistic based methods[7-9] and continuum mechanics[12-17]. Using molecular dynamics (MD), Yakobson[7] found that single-walled CNT SWNT switches into different morphological patterns under large strain and that each shape change corresponds to an sudden release of energy. Garg[8] performed MD simulation on the interactions between proximal probe guidelines composed of CNTs and diamond, and between the probe instructions and grapheme surfaces. Liew[11] studied the axial instability of SWNT and MWNTs. The atomistic based methods are currently far from predicting CNTs behavior in large length and time scales, due to insufficient computing power.[11,18] Several elasticity models can be relatively used. Ru[12] presented a shell model for the axial buckling of a double-walled CNT DWNT. He recognized a shell buckling model based on the van der Waals interaction between any two layers of MWNT. Pantano[16] presented a structural mechanics model for the wrinkling study of MWNT. Shen[17] presented an elastic shell model for the post buckling of DWNT subject to external hydrostatic pres-sure. In the above continuum models, the behavior of discrete atoms and concrete configuration of CNT in the post-buckling stage can barely be achieved. Liu[19, 20] proposed an atomic-scale finite element method AFEM. Using interatomic potential to consider the multibody interactions, AFEM is as precise as molecular mechanics. It is much faster than molecular mechanics because it uses first and second order derivatives of total energy, while molecular mechanics employs the conjugate gradient method which only uses its first order derivative.

This paper employs AFEM to study the postbuckling behavior of CNTs. The achieved energy curves and critical strain for the 8, 0 SWNT agree well with the fresh atomistic simulations. It is also found that the AFEM simulation employing the second generation empirical potential of Brenner .[21] is better than that employing Brenners first generation empirical potential.[22] In the strain energy curves for the (7,7) SWNT, there are apparent jumps at morphology changes. In the smooth continuation stages of postbuckling, the strain energy increases roughly linear. Different results on the critical strains and the postbuckling characteristics are compared and discussed for two Brenners poten-tials. For the DWNT, there are only small strain energy releases at morphology changes, and during each stage of postbuckling, the strain energy also varies roughly linear with the strain. For the SWNT and DWNT in the post-buckling stages, their morphologies are presented in detail, and the different characteristics such as the strain energy and morphologies are compared.

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Structural, spectroscopic and electrochemical study of V^{5+} substituted $LiTi_2(PO_4)_3$ solid electrolyte for lithium-ion batteries

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Abstract. Vanadium substituted $LiTi_2(PO_4)_3$ (LTP) samples of composition of $Li_{1-x}[Ti_{2-x}V_x](PO_4)_3$ ($x = 0{\cdot}0$, 0·05, 0·10 and 0·15) have been prepared by solid-state reaction method. XRD data for these compositions indicated the formation of phase pure materials of rhombohedral structure with space group $R\bar{3}c$ (167). Microstructural studies by scanning electron microscope indicated particle size in the range of 0·5–1 μm. Electrochemical impedance studies showed that ionic conductivity is high for $x = 0{\cdot}10$ composition. a.c. and d.c. conductivity results up to 573 K are in accordance with the Jonscher's power law. Cyclic voltammetry study showed its electrochemical stability in the voltage range from 0·5 to 3·5 V.

Keywords. Nasicon materials; X-ray diffraction; lithium titanium phosphate; vanadium doped $LiTi_2(PO_4)_3$.

1. Introduction

Many researchers are concentrating on finding high energy density and long life solid-state lithium-ion batteries using solid electrolytes (Birke *et al* 1999; Dhivya *et al* 2013) to power several portable electronic devices such as cell phones, laptops, digital cameras, etc (Bruce *et al* 2008; Ellis *et al* 2010; Goodenough and Kim 2010). Since no other cations except H^+ can penetrate easily into solids than Li^+, the study of rechargeable Li batteries has been actively pursued since 1970s with lithium insertion electrodes (Hong 1976; Aono *et al* 1990; Kasturi Rangan and Gopalakrishnan 1994) in the form of layered $LiCoO_2$ and spinel type $LiMn_2O_4$. On the other hand, NASICON $[Na_3Zr_2\ (SiO_4)_2(PO_4)]$ structured materials have been explored because of their high ionic conductivity, low thermal expansion coefficient and low thermal conductivity (Goodenough *et al* 1976). NASICON-type materials (isostructural with $NaZr_2(PO_4)_3$) are good ionic conductors with negligible electronic conductivity and they are stable in air (Kosova *et al* 2008). $LiTi_2(PO_4)_3$ (LTP) (Xia and Luo 2009) is one of the most promising solid electrolyte with high ionic conductivity. LTP structure is made up of two TiO_6 octahedra linked with three PO_4 tetrahedra via oxygen sharing. Lithium is present in two different types of interstitials formed by six and eight oxygen atoms, respectively. These two interstitials arranged alternatively along the conduction channels provide a three-dimensional network for Li-ion transport. In order to improve the conductivity and electrochemical properties of these materials several approaches have been developed in terms of substitution of ions such as Al, Zr, Fe, La, Mn in Ti site or by increasing Li content in the unit cell or by generating oxygen vacancies in the lattice (Kazakevicius *et al* 2008; Chen *et al* 2011). The present paper describes the effect of V^{5+} substitution in the form of $Li_{1-x}[Ti_{2-x}V_x](PO_4)_3$ on the electrochemical properties of lithium titanium phosphate material.

2. Experimental

$Li_{1-x}[Ti_{2-x}V_x](PO_4)_3$ samples with $x = 0{\cdot}0$, 0·05, 0·1 and 0·15 are synthesized by conventional solid-state reaction method. Stoichiometric amounts of Li_2CO_3, TiO_2, $NH_4H_2PO_4$ and V_2O_5 for each composition are finely ground in an agate mortar in the presence of methanol for 6 h to obtain homogeneous mixture. The powders are then calcined at 900 °C for 4 h with a heating rate of 5 °C per min. White coloured calcined powders are pressed into pellets using PVA as binder and the pellets are sintered at 1323 K for 2 h on Pt foil.

Phase identification of sintered powders has been performed on D8 ADVANCE diffractometer of BRUKER AXS with CuKα_1 radiation ($\lambda = 1{\cdot}5406$ Å) in the 2θ range from 10 to 70° in steps of 0·02°. Experimental densities of LTP and vanadium doped LTP pellets are measured at room temperature using standard Archimedes principle. Morphologies of fractured surfaces of pellets are examined with scanning electron microscopy on

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Synthesis, characterization and phase transition studies in 4-hexyloxy benzylidene 4′-alkoxyanilines

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ABSTRACT
Synthesis and the characterization through polarizing optical microscope (POM) textures in number of 4-hexyloxy benzylidene 4′-alkoxyanilines, 6O.O*m* with *m* = 4, 6 to 10 liquid crystalline materials are carried out. Furthermore, the density and thermal expansion coefficient results reveal that the phase transitions present, viz., isotropic–nematic, nematic–SmC and SmC–SmI show first-order nature as expected. The transition temperatures obtained thorough the differential scanning calorimetry is found to be in agreement with the literature data. The first two compounds exhibit only the nematic phase while the next four compounds show enantiotropic SmC phase as per the literature data. The compound with *m* = 10 exhibits monotropic SmI phase. However, we, the authors, are able to observe this phase in addition to SmC and nematic through POM only as per the literature. The parameters calculated across the phase transitions and in the phases are in agreement with the body of the data available.

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4-hexyloxy benzylidene 4′-alkoxyanilines; POM; phase transitions; density studies; DSC; order of the transitions

Introduction

The liquid crystals (LCs) are mysterious materials and they differ from the solids and isotropic compounds. These materials possess both flow as well as anisotropic properties. Therefore, they are being used in many applications.[1–4] The density results also will provide the information regarding the nature of phase transitions across different LC phases as well as in between the isotropic to LC phase. The *n*O.*m* compounds have the unique nature of exhibiting a variety of polymorphism. The systematic studies and the literature data [5] reveal that these compounds exhibit 21 different types of phase variants starting from mono variant (N or A) to hexa variant (NACBFG). The compounds with less number of carbon atoms in alkyl chains exhibit nematic and smectic-A phases with few exceptions.[5] Systematic studies and the literature data [6–10] on the compounds *n*O.O*m* (to which these two compounds belong) reveal that these exhibit 13 different phase variants starting from mono variant (N, A or C) to penta variant (NACIG). The compounds under study belong to this homologous series. The systematic studies reveal that the change in the position of oxygen on either side of the rigid core (benzylidene aniline group) affects the phase transitions. (1) If the oxygen is on the benzaldehyde side, the compound exhibits to be rich in polymorphism (4O.4 and 5O.5). This is, the trend that has been observed from the systematic studies have been carried out on *n*O.*m* compounds. (2) If the oxygen is on the aniline side, the intermediate smectic phases are quenched with no considerable change in the clearing temperature. (3) When the oxygen is on

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Estimation of thermodynamic parameters in 4-(hexyloxybenzylidene)-4′alkoxy anilines, 6O·Om liquid crystalline compounds – A density study

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ABSTRACT

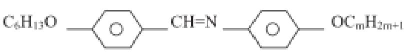
The various thermodynamic parameters such as Sharma parameter (S_o), Huggins parameter (F), reduced volume ($\tilde{V}$), reduced compressibility ($\tilde{V}^{C1}$), etc. are studied for the homologues series of 4-(hexyloxybenzylidene)-4′ alkoxy anilines, 6O·Om liquid crystalline (LC) compounds with m = 4 to 10 by employing thermal expansion coefficient obtained from density variation with temperature in isotropic and liquid crystalline phases. In addition to these, molecular radius (from refractive index) and the Beyer's non linearity parameter, B/A are estimated. All the parameters are in agreement with the other reported liquid crystalline compounds, liquids and polymers and the data obtained is compared with the literature data available.

1. Introduction

Systematic studies and the literature data [1–4] on the nO·Om compounds reveal that these class of compounds exhibit 13 different phase variants starting from mono variant (N, A, or C) to penta variant (NACIG). Further, it is observed from the systematic studies on the Schiff's base compounds that the position of the oxygen atom in the molecular moiety plays an important role in deciding the clearing temperature the richness of the nematic phase and the phase variant a compound exhibits. The study of internal structure and thermodynamical behavior of the Liquid Crystal (LC) molecule is also important to understand the behavior of the material. In the present investigation it is proposed to estimate thermo dynamic parameters and the anharmonic parameters such as the isochoric temperature coefficient of internal pressure (X), isochoric temperature coefficient of volume expansivity (X′), the reduced compressibility ($\tilde{\beta}$), the reduced volume ($\tilde{V}$), isothermal microscopic Gruneisen parameter (Γ), fractional free volume (f) and Sharma parameter (S_0) are estimated from the data of the coefficient of volume expansion in the isotropic and liquid crystalline phases. The temperature dependence of these parameters may give a basic understanding about the molecular order and intermolecular interactions in the condensed matter. In the present manuscript we attempted to estimate the thermodynamic parameters in homologues series of 4-hexyloxybenzylidene)-4′-alkoxy anilines, 6O·Om liquid crystalline compounds with m = 4 to 10 in isotropic and liquid crystalline phases.

2. Experimental

The molecular formula of the compounds is given below:



where m = 4 to10.

The present compounds are synthesized following the established procedure reported in the literature [5]. The transition temperatures and the enthalpy values obtained from Perkin-Elmer diamond DSC, the textures as well as the transition temperatures are identified by using polarizing microscope attached with an indigenous hot stage. The temperature resolution of the microscopic studies is ±0.1 °C. The density measurements are carried out using a bicapillary pycnometer. The capillary diameter of the pycnometer is of the order of 3.5×10^{-4} m and accuracy in density measurements is ±0.1 kg m^{-3}. The permitted cooling rate was 1 °C per hour and temperature accuracy is ±0.1 °C. The details of all these were reported in our recent publication [6].

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ESTIMATION OF ORIENTATIONAL ORDER PARAMETER FROM DIFFERENT MODELS IN 6O.Om LC MATERIALS - AN OPTICAL STUDY

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Abstract

The refractive indices measurements are carried out on a number of Schiff's base 6O.Om compounds with m = 4, 6 to 10 using a wedge shaped cell with a modified spectrometer. The transition temperatures obtained using the POM and DSC are in agreement within the experimental errors. The birefringence data $\delta n = (ne - no)$ along with the density results are employed to estimate the molecular polarisabilty anisotropy, $\delta\alpha = (\alpha e - \alpha o)$ assuming a particular local field (due to Vuks and Neugebauer) the nematic molecule experiences and the order parameter S is estimated from $\delta\alpha$ and $\Delta\alpha$, i.e., polarisabilty anisotropy in the perfect order which is estimated employing different methods. Using these values, the orientational order parameter S has been estimated at

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Keywords and phrases: Schiff's base 6O.Om LC compounds, refractive indices, orientational order parameter, molecular polarizabilities.
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