

## Curriculum Vitae



**Israel Samuel Ph.D.**

Name	: Dr. S. Israel
Nationality	: Indian
Date of Birth	: 21 <sup>st</sup> May 1968
Address	: 2/492, Bagath Singh Nagar 7 <sup>th</sup> Street, Kadachanendal, Madurai – 625002, Tamil Nadu, India
Institution	: Department of physics, The American College, Madurai – 625 002, Tamil Nadu, India
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Scholarly reference	: <a href="https://www.researchgate.net/profile/Israel_Samuel">https://www.researchgate.net/profile/Israel_Samuel</a> <a href="https://www.mendeley.com/profiles/israel-samuel/">https://www.mendeley.com/profiles/israel-samuel/</a> <a href="https://orcid.org/0000-0002-6294-351X">https://orcid.org/0000-0002-6294-351X</a>
URL	: <a href="https://israelsamuel.weebly.com">https://israelsamuel.weebly.com</a>

### **Education:**

- Bachelor of Science, Physics Major, The American college, Madurai, Tamil Nadu, India, 1988
- Master of Science, Physics Major, NMSSVN college, Madurai, Tamil Nadu, India, 1990
- Master of Philosophy in Physics, Madurai Kamaraj University, Madurai, Tamil Nadu, India, 1991
- Doctor of Philosophy in Physics, Madurai Kamaraj University, Madurai, Tamil Nadu, India, 2005

### **Areas of Interest:**

- Crystallography and crystal structures
- Charge density in
  - Semiconductors and their properties
  - Diluted Magnetic Semiconductors
  - Minerals, Oxides, Fluorides and Oxyfluorides
  - Pharmaceutically important materials
- Charge density analysis and their topology
- Quantum chemical calculations from charge density
- Nanomaterial preparation and characterization
- Single crystal and poly-crystal preparation and characterization

- Correlating electric/magnetic behaviour of solids with the rearrangement of charges between the atoms and in the unit cell.
- Correlating the inclusion of impurities and the change in the charge environment of the atoms and then to the change in their physical and chemical properties.
- Correlating the interaction between the molecules preferably between the pharmaceutical and amino acid systems and with their implications on the curing process.
- Understanding the physical changes in the mineral systems due to thermal and pressure variations.
- Understanding Oxygen, fluorine binding with various groups of atoms in the periodic table
- Analysing Phase transition and Polymorphism using charge density route

### **Professional Positions held:**

- Lecturer in Physics, NMSSVN college, Madurai, Tamil Nadu, India, 1992-95
- Lecturer in Physics, Christ Church college, Kanpur, UP, India, 1995-2001
- FDP substitute (Lecturer in Physics), The American college, Madurai, Tamil Nadu, India, Dec 2004 – March 2007
- Lecturer in Physics, The American college, Madurai, Tamil Nadu, India, 2001 – July 2001 – Nov 2004, April 2007- Sept 2007.
- Assistant Professor in Physics, The American college, Madurai, Tamil Nadu, India, Sept 2007 – Oct 2019
- Associate Professor in Physics, The American college, Madurai, Tamil Nadu, India, Nov 2019 – till date

### **Professional Body:**

- Board of studies member in
  - The Madura College, Madurai, Tamil Nadu, India
  - Yadava college, Madurai, Tamil Nadu, India
  - Kalasalingam University, Krishnankoil, Tamil Nadu, India
- Life member in “Indian Crystallography association”
- Life member in “All India Association for Christian Higher Education (AIACHE)”

### **Awards:**

- Awarded three R&D fellowships funded by **The American College, Madurai, India**
- Awarded Major Research Fellowship by **University Grant Commission, India** for a project on “Quantifying electrostatic potential of some pharmacologically important compounds” in the year 2012-15 for an award of Rs. 12lakhs
- Awarded **Defence secretary's commendation** for outstanding leadership in NCC for the year 2014
- **Summer Research Fellowships** – 2014 awarded by Indian Academy of sciences and worked on a project titled “Enhancing Physical stability of

silicon clusters by doping: A Density functional Theory based approach” –  
Reg. No: PHYT 105

**Editorial Board Member:**

- ❖ Journal of Material Science: Materials in Electronics; Springer Publications, Springer Nature Switzerland AG.

**Reviewer board member:**

**Completed Assignments Total = 63**

- ✓ Journal of Material Science: Materials in Electronics; Springer Publ. -38
- ✓ Material science in semiconductor processing ; Elsevier Publications-10
- ✓ Materials Chemistry and Physics - Journal - Elsevier Publications -5
- ✓ Results in Physics - Journal - Elsevier Publications - 3
- ✓ Physica B: Condensed Matter Physics - Elsevier Publications- 1
- ✓ European Journal of Chemistry -Atlanta Publishing House LLC, USA- 1
- ✓ Journal of Material Science & Engineering- Springer Nature - 1
- ✓ Luminescence: The Journal of Biological and Chemical luminescence, John Wiley & Sons-1
- ✓ Materials today: Proceedings, Elsevier publications -2
- ✓ Journal of The Australian Ceramic society (Springer - Nature) - 1

**Administrative Positions held:**

- NCC: Associate NCC Officer of rank Lt. Cdr (Navy) from 2003-2020 (17 years)
- Additional Dean of Self Financed Courses from 2012-2020( 8 years)
- Additional Dean of Curriculum development and research from 2020
- Faculty secretary for 2019 - 2020
- Governing council member of The American college, Madurai from 2019-21

**Co-curricular activities:**

- Commissioned as an NCC (Navy) officer in 2003 and elevated to the rank of Lieutenant Commander in 2018 and as the sub unit commander (NCC NAVY) at The American College, Madurai.
- Taught courses on Photography, “How things work”, “Physics of Home appliances” as selective subjects for under graduate students.

**Research supervision:**

- PhD Supervision
  - Total Number of students - 7          Students completed PhD - 4
- MPhil Students completed - 37

## List of Published research works

### Total Number of Publications: - 62

62

Structure, Charge density and Hirshfeld Surface Analysis of proton transfer complex 2-Amino-4-methylpyridinium 2-(3-methylphenyl)-acetate

C.Anzline, **S.Israel**, K.Sujatha and R.A.J.R.Sheeba

Journal of the Chinese Chemical Society(Wiley), **1-14, 2022**

DOI:10.1002/jccs.202100433

61

Three dimensional atomistic-scale electron density distribution analysis of ZnWO<sub>4</sub>: Sm phosphors

S. Saravanakumar, D. Sivaganesh, V. Sivakumar, Yang Li, Rajajeyaganthan Ramanathan, **S. Israel**

**Optik :International Journal for Light and Electron Optics(Elsevier):249, January**

**2022, Available online 15 October 2021, 168169**

DOI: <https://doi.org/10.1016/j.ijleo.2021.168169>

60

Charge density of difluorides from synchrotron diffraction data and investigation of bonding in low valent binary fluorides

K.Sujatha, **S.Israel**, C.Anzline, R.A.J.R.Sheeba

**Materials Chemistry and Physics 259 (2021) 123990**

<https://doi.org/10.1016/j.matchemphys.2020.123990>

59

Hirshfeld Surface, Charge Density and Site Selectivity Studies of 1-(2-Methyl-5-nitro-1H-imidazol-1-yl)-acetone

C.Anzline, **S.Israel**, K.Sujatha and R.A.J.R.Sheeba

**Computational and Theoretical Chemistry 1191 (2020) 113044**

<https://doi.org/10.1016/j.comptc.2020.113044>

58

A theoretical study of chemical bonding and topological and electrostatic properties of the anti-leprosy drug dapsone

Niranjana Devi Rajendran, Natarajan Mookan, **Israel Samuel**, Sarath Babu Mookan, Govindarajan Munusamy, Selvaraj Gurudeeban, Satyavani Kaliamurthi

**Journal of Molecular Modeling (2020) 26:138**

<https://doi.org/10.1007/s00894-020-04393-6>

57

Experimental validation of bifurcated hydrogen bond of 2,5-lutidinium bromanilate and its charge density distribution

Niranjana Devi Rajendran, Natarajan Mookan, **Israel Samuel**, Sarath Babu Mookan

**Chemical Papers, volume 74(2020)2689–2699**

<https://doi.org/10.1007/s11696-020-01107-3>

56

Aceclofenac and interactions analysis in the crystal and COX protein active site

Christian Jelsch, Rajendran Niranjana Devi, Bruce C. Noll, Benoît Guillot, **Israel Samuel**, Emmanuel Aubert

**Journal of Molecular Structure 1205 (2020) 127600**

<https://doi.org/10.1016/j.molstruc.2019.127600>

55

X-ray derived experimental charge density distribution in two isostructural oxyfluorotellurates, FeTeO<sub>3</sub>F and GaTeO<sub>3</sub>F

K. Sujatha, **S. Israel** and C. Anzline

**Physica B: Condensed Matter**, **579** (2020) 411896

<https://doi.org/10.1016/j.physb.2019.411896>

**54**

Comprehensive study on the topological properties of 5-Amino-2-Methyl Benzene Sulfonamide involving inter and intra molecular hydrogen bonds

C. Anzline, P. Sivakumar, **S. Israel**, K. Sujatha

**Journal of Molecular Structure** **1201** (2020) 127208

<https://doi.org/10.1016/j.molstruc.2019.127208>

**53**

Origin of ferroelectricity in orthorhombic LuFeO<sub>3</sub>

Ujjal Chowdhury, Sudipta Goswami, Amritendu Roy, Shailendra Rajput, A. K. Mall, R.

Gupta, S. D. Kaushik,

V. Siruguri, S. Saravanakumar, **S. Israel**, R. Saravanan, A. Senyshyn, T. Chatterji, J. F. Scott, Ashish Garg, and Dipten Bhattacharya

**PHYSICAL REVIEW B** **100**, 195116 (2019)

DOI: 10.1103/PhysRevB.100.195116

**52**

Photoluminescence study of (Sm<sub>0.95</sub> Ce<sub>0.05</sub>)<sub>2</sub>O<sub>3</sub> nanoparticles for LED applications

MM Antoinette, S Israel, JL Berchmans, AJ Amali

**AIP Conference Proceedings** **2162** (1), 020116, 2019

**51**

Analysis of oxygen bonding with metals of different oxidation states from experimental charge density distribution

K. Sujatha, **S. Israel**, C. Anzline, K.S. Syed Ali, R.A.J.R. Sheeba, P. Richard Rajkumar

**Physica B: Condensed Matter** **555** (2019) 21–31

<https://doi.org/10.1016/j.physb.2018.12.005>

**50**

Enhanced photoluminescence and charge density studies of novel (Sm<sub>1-x</sub> Gdx)<sub>2</sub>O<sub>3</sub> nanophosphors for WLED applications

Morris Marieli Antoinette, **S. Israel**, John L. Berchmans & G. J. Manoj

**Journal of Materials Science: Materials in Electronics** (2018) **29**:19368–19381

<https://doi.org/10.1007/s10854-018-0066-1>

**49**

Investigation of topological and electrostatic properties of anti-inflammatory drug aceclofenac

Niranjana Devi Rajendran, Christian Jelsch, **Israel Samuel** and Emmanuel Aubert

**Acta Crystallographica Section A: Foundations and Advances** **73(a2)**:C698-C698, December 2017,

DOI :10.1107/S2053273317088751

**48**

A novel synthesis of orange-red emitting (Sm<sub>1-x</sub>Cex)<sub>2</sub>O<sub>3</sub> nanophosphors for UV LEDs

Morris Marieli Antoinette, **S. Israel**, Arlin Jose Amali, John L. Berchmans, Basuvaraj Suresh Kumar, G.J. Manoj and U. Mehana Usmania

**Nano-Structures & Nano-Objects** **13** (2018) 51–58

**47**

Crystal structures of 2-methylpyridinium hydrogen 2,3-bis(4-methylbenzoyloxy)succinate and bis-[4-methylpyridinium hydrogen 2,3-bis(4-methylbenzoyloxy)succinate] pentahydrate

P. Sivakumar, **S. Israel** and G. Chakkaravarthi

**Acta Cryst. (2017). E73, 1483–1487**

**46**

Understanding electronic and magnetic transitions in ball milled diluted magnetic semiconductor Si<sub>1-x</sub>Ni<sub>x</sub> through experimental electron density distribution

R.A.J.R. Sheeba, S. Saravanakumar, **S. Israel**, R. Saravanan

**Journal of Alloys and Compounds 728 (2017) 887-895**

**45**

Experimental charge density distribution and its correlation to structural and optical properties of Sm<sup>3+</sup> doped Nd<sub>2</sub>O<sub>3</sub> nanophosphors

Morris Marieli Antoinette, **S. Israel**, G. Sathya, Arlin Jose Amali, John L. Berchmans, K. Sujatha, C. Anzline and R.Niranjana Devi

**Journal of Rare Earths 35 (2017) 1102 -1114**

**44**

Testing the ability of rhodanine and 2, 4-thiazolidinedione to interact with the human pancreatic alpha-amylase: electron-density descriptors complement molecular docking, QM, and QM/MM dynamics calculations

R. Niranjana Devi, Maria G. Khrenova, **S. Israel**, C. Anzline, Andrey A. Astakhov, Vladimir G. Tsirelson

**Journal of Molecular Modelling 23(2017) 252**

**43**

2-Amino-4-methylpyridinium 4-methoxybenzoate dihydrate

P. Sivakumar, G. Ezhamani, **S. Israel** and G. Chakkaravarthi

**IUCrData (2017). 2, x170649**

**42**

2-Amino-3-methylpyridinium hydrogen phthalate

P. Sivakumar, C. Anzline, S. Sudhahar, **S. Israel** and G. Chakkaravarthi

**IUCrData (2017). 2, x170422**

**41**

Charge density analysis of Metformin/HCl, a biguanidean anti-hyperglycemic agent

R. Niranjana Devi, C. Jelsch, **S. Israel**, E. Aubert, C. Anzline and A. A. Hosamani

**Acta Crystallographica Section B:**

**STRUCTURAL SCIENCE, CRYSTAL ENGINEERING AND MATERIALS,(2017).**

**B73, 10-22**

**40**

High Resolution Synchrotron Diffraction Study on Charge Density Distribution of Ampicillin Trihydrate: A Correlation between DFT and Multipole Models

C. Anzline, **S. Israel**, R. Niranjana Devi, R.A.J.R. Sheeba and P. Richard Rajkumar

**Chinese Journal of Chemical Physics VOLUME 30, NUMBER 1,2017(Thomson Reuters)**

**39**

2-Amino-4-methylpyridinium 2-hydroxybenzoate

P. Sivakumar, **S. Israel** and G. Chakkaravarthi

**IUCr Data, Data reports Vol.1,Part 4 (2016)x161443**

**38**

2-(4-Nitrophenyl)acetate 2-amino-4-methylpyridin-1-ium

P. Sivakumar, C. Anzline, **S. Israel** and G. Chakkaravarthi

**IUCr Data, Data reports Vol.1,Part 4 (2016)x161433**

**37**

2-Amino-4-methylpyridinium 4-hydroxybenzoate

- P. Sivakumar, S. Sudhahar, **S. Israel** and G. Chakkaravarthi  
**IUCr Data, Data reports Vol.1,Part 4 (2016)x161425**  
**36**  
2-Amino-4-methylpyridinium 4-methylbenzoate  
P. Sivakumar, C. Anzline, **S. Israel** and G. Chakkaravarthi  
**IUCr Data, Data reports Vol.1,Part 4 (2016)x161411**  
**35**  
2-Amino-3-methylpyridinium 3,4-dimethoxybenzoate  
P. Sivakumar, R. Niranjana Devi, **S. Israel** and G. Chakkaravarthi  
**IUCr Data, Data reports Vol.1,Part 4 (2016)x161332**  
**34**  
Investigation on van der Waals epitaxy gap in isostructural semiconducting germanium  
Tellurides: HfGeTe<sub>4</sub> and ZrGeTe<sub>4</sub>  
R. A. J. R. Sheeba, **S. Israel** and S. Saravanakumar  
**Chinese journal of physics(Elsevier)54 (2016) 668–677**  
**33**  
Bis(2-amino-6-methylpyridinium) 3-nitrobenzene-1,2-dicarboxylate  
P. Sivakumar, S. Sudhahar, **S. Israel** and G. Chakkaravarthi  
**IUCr Data, Data reports Vol.1,Part 4 (2016)x161233**  
**32**  
2-Amino-4-methylpyridinium 2-(4-nitrophenyl)-acetate  
P. Sivakumar, S. Sudhahar, **S. Israel** and G. Chakkaravarthi  
**IUCr Data, Data reports Vol.1,Part 4 (2016)x161203**  
**31**  
2-Amino-3-methylpyridinium 4-methoxybenzoate  
P. Sivakumar, R. Niranjana Devi, **S. Israel** and G. Chakkaravarthi  
**IUCr Data, Data reports Vol.1,Part 4 (2016)x161126**  
**30**  
2-Methylpyridinium 2-carboxy-6-nitrobenzoate  
Sivakumar, P., Sudhahar, S., **Israel, S.** and Chakkaravarthi, G.  
**IUCr Data, Data reports Vol.1,Part 4 (2016)x161104**  
**29**  
2-Amino-4-methylpyridinium 2-(3-methylphenyl)-acetate  
Sivakumar, P., Sudhahar, S., **Israel, S.** and Chakkaravarthi, G.  
**IUCr Data, Data reports Vol.1,Part 4 (2016)x161098**  
**28**  
3-Methylpyridinium 4-nitrobenzoate–4-nitrobenzoic acid(1/1)  
P. Sivakumar, R. Niranjana Devi, **S. Israel** and G. Chakkaravarthi  
**IUCr Data, Data reports Vol.1,Part 4 (2016)x160979**  
**27**  
X-ray derived experimental charge density distribution in GaF<sub>3</sub> and VF<sub>3</sub> solid systems  
K.Sujatha , **S. Israel** , C.Anzline, R.Niranjana Devi and R.A.J.R.Sheeba.  
**Physica B: Condensed Matter 496(2016)74–81.**  
**26**  
Piperazin-1-ium 4-aminobenzoate monohydrate  
P. Sivakumar, A. Mani, S. Sudhahar, **S. Israel** and G. Chakkaravarthi  
**IUCr Data, Data reports Vol.1,Part 4 (2016) x160819.**  
**25**  
2-Methylpyridinium 2-carboxybenzoate–benzene-1,2-dicarboxylic acid (2/1)  
P. Sivakumar, S. Sudhahar, B. Gunasekaran, **S. Israel** and G. Chakkaravarthi

**IUCr Data, Data reports Vol.1,Part 4 (2016) x160817.**

**24**

2-Amino-6-methylpyridinium 2-hydroxybenzoate

P. Sivakumar, S. Sudhahar, **S. Israel** and G. Chakkaravarthi

**IUCr Data, Data reports Vol.1,Part 4 (2016) x160747.**

**23**

4-Aminobenzoic acid–quinoline (1/1)

P. Sivakumar, S. Sudhahar, **S. Israel** and G. Chakkaravarthi

**IUCr Data, Data reports Vol.1,Part 4 (2016) x160604.**

**22**

Structure and stability of a silicon cluster on sequential doping with carbon atoms

Mohammed Azeezulla Nazrulla, Krati Joshi, **S. Israel** and Sailaja Krishnamurthy

**Physica E: Low-dimensional Systems and Nanostructures, 76 (2016)173–180**

**21**

Structural, magnetic and charge-related properties of nano-sized cerium manganese oxide, a dilute magnetic

oxide semiconductor

S. Saravanakumar, S. Sasikumar, **S. Israel**, G.R. Pradhiba, R. Saravanan

**Materials Science in Semiconductor Processing 17 (2014) 186–193**

**20**

The analysis on the rearrangement of charge density distribution in response to magnetic behavior in Mn doped SnO<sub>2</sub> nanoparticles

S. Saravanakumar, M. Pattammal, **S. Israel**, R.A.J.R.Sheeba, R. Saravanan,

**Physica B: Condensed matter physics, 407 (2012) 302.**

**19**

Analysis on insulator-metal transition in Yttrium doped LSMO from electron density distribution

**S. Israel**, S. Saravana Kumar, A. Renuretson, R. A. J. R. Sheeba, R. Saravanan,

**Bulletin of Material science, Vol.35.No.1 (2012) 111.**

**18**

Localized ferromagnetic charge ordering through charge density analysis in nano sized diluted magnetic semiconductor Co<sub>2+</sub>:ZnO

K.S. Syed Ali, R. Saravanan, **S. Israel**, M. Açıkgöz, L. Arda,

**Physica B:Condensed matter Physics 405 (2010) 1763–176.**

**17**

Analysis on experimental valence charge density in Germanium at RT and 200 K

**S. Israel**, K.S. Syed Ali, R. A. J.R. Sheeba and R. Saravanan

**Journal of Physics and Chemistry of Solids 70 (2009) 1185–1194**

**16**

Growth of novel diluted magnetic semiconducting material Ge<sub>1-x</sub>Mn<sub>x</sub> and X-ray characterization by Maximum Entropy Method (MEM) and Pair Distribution Function (PDF)

R Saravanan, K. S. Syed Ali and **S. Israel**

**Journal of Crystal Growth 311 (2009) 1110–1116.**

**15**

X-ray analysis of charge density distribution in GaP at 296 and 200K using Multipole and MEM models

**S. Israel**, K.S. Syed Ali, R.A.J.R. Sheeba and R. Saravanan

**Chinese Journal of Physics 47, 3(2009) 378-400**

**14**

Electron density distribution in Si and Ge using multipole, maximum entropy method and



pair distribution function.

R Saravanan, K. S. Syed Ali and **S. Israel**  
**Pramana – Journal of Physics, 70, 4,(2008).**

**13**

Probabilistic Electron Density Distribution in CdTe at 200 K and 300 K.

R. Saravanan, **S. Israel**, R. K. Rajaram, Y. Ono, M . Isshiki and T. Kajitani.

**Crystal Research and Technology 3, 41, (2006)**

**12**

Electron density distribution and bonding in ZnSe and PbSe using maximum entropy method (MEM)

K. S. Syed Ali, R. Saravanan, **S. Israel**, R. K. Rajaram

**Bulletin of Materials Science, 29, No.2, 107-114, Apr.2006**

**11**

Bonding in ZnTe at RT, 200 and 100 K Revealed by Entropy Maximized Electron Density Distribution.

R. Saravanan, **S. Israel** and R. K. Rajaram

**Physica B: 363/1-4,166-177, 2005**

**10**

Bonding in Fluorite Compound CaF<sub>2</sub> Using MEM.

R. Saravanan and **S. Israel**.

**Physica B: 352/1-4, 220-226, (2004).**

**9**

Electronic Structure of InP at RT, 200K and 100K.

**S. Israel**, R. Saravanan, and R.K. Rajaram.

**Physica B: 349, 390-400, (2004).**

**8**

An investigation on the bonding in MgO, CaO, SrO and BaO from the MEM electron density distributions

**S. Israel**, R . Saravanan, N. Srinivasan and S.K. Mohanlal

**Journal of Physics and Chemistry of Solids, 64, 879-886, (2003).**

**7**

Electronic Charge Distribution in the Intermetallic Compound MnHg

R. Saravanan, **S. Israel**, S. Swaminathan, R. Kalidoss and M. Muruganantham

**Crystal Research and Technology, 37, Issue 12, 1310-1317, (2002)**

**6**

High Resolution Electron Density Mapping for LiF and NaF by Maximum Entropy Method (MEM)

**S. Israel**, R. Saravanan, N.Srinivasan, R. K. Rajaram

**Journal of Physics and Chemistry of Solids, 64/1, 43-49, (2002).**

**5**

X-ray structure of BaTiO<sub>3</sub>-Missed Opportunities

K. S. Chandrasekaran, S. K. Mohanlal, R. Saravanan, **S. Israel**

**Acta Crystallographica, B56, 918-919, (2000)**

**4**

Charge transfer in GaP and InP

R. Saravanan, **S. Israel**, N. Srinivasan, and S. K. Mohanlal

**Phys. Status Solidi B (Germany), vol.194, no.2, 435-41, 1 APRIL, (1996), Akademie Verlag**

**3**

Charge transfer in ZnSe

N. Srinivasan, R. Saravanan, **S. Israel**, and S. K. Mohanlal  
**Cryst. Res. Technol. (Germany), vol.31, no.1, K6-8, (1996), Akademie Verlag**

**2**

Debye-Waller factors in  $\text{Na}_x\text{C}_{60}$

N. Srinivasan, R. Saravanan, **S. Israel**, and S. K. Mohanlal  
**Cryst. Res. Technol. (Germany), vol.30, no.3, K37-9, (1995)**

**1**

$f''$  of silicon from linear absorption measurements

N. Srinivasan, **S. Israel**, R. Saravanan, and S. K. Mohanlal  
**Cryst. Res. Technol. (Germany), vol.30, no.1, K1-3, (1995)**

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### List of papers presented in Symposium/ Seminar/ Conference/ Workshop

#### Total number of papers presented: - 46

**46**

Photoluminescence study of  $(\text{Sm}_{0.95}\text{Ce}_{0.05})_2\text{O}_3$  nanoparticles for LED applications  
Morris Marieli Antoinette, **S. Israel**, John L. Berchmans, and Arlin Jose Amali  
AIP Conference Proceedings 2162, 020116 (2019); <https://doi.org/10.1063/1.5130326>

**45**

Structure And Site Selectivity Studies of Non Steroidal Anti Inflammatory Drug Ibuprofen  
using DFT Technique

C. Anzline, **S. Israel**, K. Sujatha

International conference on innovation and sustainable development of science, social science,  
management and technology (ISDSSMT- 19), DMI-St. Eugene University, Lusaka, Zambia,  
South- Central Africa. ISBN: 978-81-940502-3-0

**44**

X-Ray Derived Experimental Charge Density Distribution in Transition Metal

Oxyfluorotellurate:  $\text{GaTeO}_3\text{F}$

K. Sujatha, **S. Israel**, C. Anzline

International conference on innovation and sustainable development of science, social science,  
management and technology (ISDSSMT- 19), DMI-St. Eugene University, Lusaka, Zambia,  
South- Central Africa. ISBN: 978-81-940502-3-0

**43**

X-ray Analysis of the Charge Density Distribution in Transition Metal Oxyfluorotellurate:  
 $\text{FeTeO}_3\text{F}$

K. Sujatha, **S. Israel**, C. Anzline

International Conference on Recent Advances in Material Sciences, 4 – 6 February 2019,  
National College (Autonomous), Thiruchirapalli, Tamil Nadu.

**42**

Molecular Structure and site selectivity studies in N- Methyl – N- nitroso – p- toluene  
sulfonamide using DFT Technique

C. Anzline, **S. Israel**, K. Sujatha

International Conference on Recent Advances in Material Sciences, 4 – 6 February 2019,  
National College (Autonomous), Thiruchirapalli, Tamil Nadu.

**41**

Photoluminescence studies of  $(\text{Nd}_{0.93}\text{Sm}_{0.07})_2\text{O}_3$  Nanoparticles

Morris Marieli Antoinette, **S. Israel**

International conference of advanced materials 14 - 15 December, 2017

St. Josephs college, Trichy.

**40**

Investigation on the properties of Sm<sup>3+</sup>-doped Nd<sub>2</sub>O<sub>3</sub> nanoparticles and X-ray characterization by the maximum entropy method (MEM)

Morris Marieli Antoinette, **S. Israel**, G. Sathya, Arlin Jose Amali, John L. Berchmans, K. Sujatha and C. Anzline

Fourth International Conference on Nanostructured Materials and Nanocomposites (ICNM 2017) on 10, 11 and 12 February 2017 at Mahatma Gandhi University, Kottayam, Kerala, India

**39**

An analysis of structural, electronic and reactivity properties of Metformin Chloride using XRD and DFT approach

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