



# NANJIL CATHOLIC COLLEGE OF ARTS AND SCIENCE

Kaliyakkavilai, Kanyakumari District - 629153

Accredited by NAAC with 'B' Grade

(Approved by the Govt. of Tamil Nadu and Affiliated to Manonmaniam Sundaranar University, Tirunelveli)

## FOURTH NATIONAL CONFERENCE ON ADVANCED MATERIALS

(NCAM-2022)

March 26, 2022



This is to certify that Mr./Ms./Dr. **RATHIKA A.** Assitant..... Professor.....  
.....**Masilu Arts College, Tiruvithirai**..... has attended the Fourth

National Conference on Advanced Materials (NCAM-2022) organized by the  
Department of Physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai on

March 26, 2022 and presented a paper (Poster/Oral) entitled **Single crystal growth and optical properties of glutaric acid doped polyacrylonitrile hydrogen phthalate single crystals**

Rev. Fr. Dr. M. Pergrandy Michael

Secretary and Correspondent

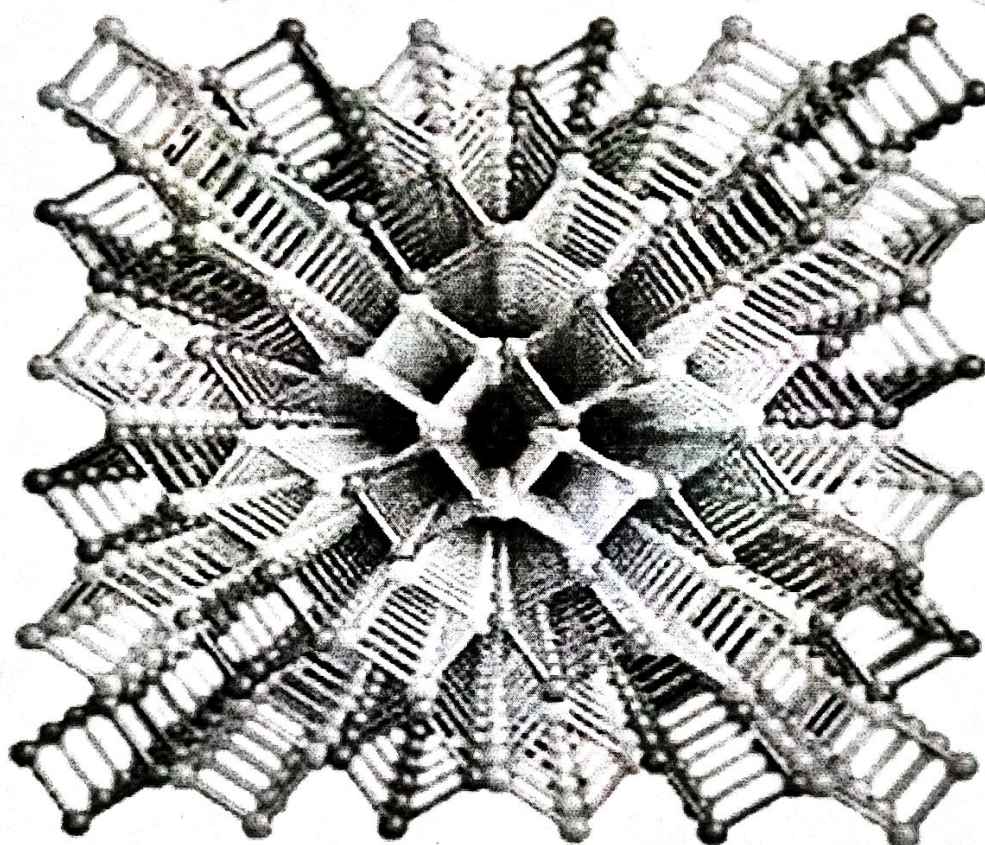
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**Fourth National Conference  
on  
ADVANCED MATERIALS  
(NCAM- 2022 )**



**Conference Proceeding**

**Edited by**

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**Nanjil Catholic College of Arts and Science  
Kaliyakkavilai**

**NANJIL CATHOLIC COLLEGE OF ARTS AND SCIENCE**

**KALIYAKKAVILAI**

**(APPROVED BY THE GOVERNMENT OF TAMIL NADU**

**AND AFFILIATED TO MANONMANIAM SUNDARANAR UNIVERSITY, TIRUNELVELI)**

**ACCREDITED BY NAAC WITH 'B' GRADE**

**APPROVED BY UGC NEW DELHI UNDER THE SECTION OF 2(F) AND 12(B) OF THE UGC ACT.1956**



**Editor**

**Dr.M.Amalanathan**

**Assistant Professor, Department of Physics  
Nanjil Catholic College of Arts and Science**

**Email: [nathan.amalphysics@gmail.com](mailto:nathan.amalphysics@gmail.com)**

**Mobile: 9940347178**



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14. Vibrational spectroscopic characterization, DFT studies and structural investigations of N-(2-Hydroxybenzylidene)-2-Iodoaniline (D.Jayareshmi<sup>1,\*</sup>, D.Aruldas<sup>2,\*</sup>)
15. Vibrational and Optical Studies of 3,4,5-trimethoxybenzaldehyde single crystals for NLO applications (R.P. Jebin<sup>a</sup> and T. Suthan<sup>b</sup>)
16. Vibrational spectral investigation, DFT computational studies and charge transfer interactions analysis of l-lysine monohydrate (T. Brintha<sup>1</sup>, J. Jeni James<sup>2</sup>, P.J. Jegan Babu<sup>3</sup>, M. Amalanathan<sup>4</sup>)
17. Structural, computational, C-H...O/N-H...O hydrogen bonding, homo-lumo, mesp and nbo analysis of n-2(hydroxy phenyl) acetamide (M.Jini pramila<sup>1</sup>, D.Arul Dhas<sup>2,\*</sup>)
18. Single crystal growth and optical properties of glutaric acid doped potassium hydrogen phthalate single crystals (A. Rathika<sup>a</sup>, R.Ganapathi Raman<sup>\*</sup>)
19. Effect of metal doping on the properties of SnO<sub>2</sub> nanoparticles (T.Regina Das<sup>1, 2</sup>, M. Meena<sup>3,\*</sup>)
20. Periodic variations of sunspot activities in 24<sup>th</sup> solar maximum (Mariya Shaniya.S<sup>1\*</sup>, Iren Sobia.A<sup>2</sup>)
21. Synthesis and optical characterization of creatinium 5- sulfosalicylate (S.S.Sherlin<sup>a</sup>, C.Christal Vasanthi<sup>b\*</sup>, S.Sindhusha<sup>b</sup>)
22. Theoretical and spectroscopic studies of orotic acid (S.Sijana<sup>1</sup>, M. Amalanathan<sup>2</sup>)
23. Crystal growth, XRD and vibrational studies of piperazine p-nitrophenol (ppn) single crystals (R.Suja<sup>a</sup>, A.Rathika<sup>\*</sup>)
24. Structural characterization of Zn and Fe doped aluminium oxide nanoparticles prepared by co-precipitation method (R.Winston<sup>(1)</sup>, T.R Jeena<sup>(2)</sup>)
25. Synthesis and Characterization of Cu-Doped ZnSe Nanoparticles for Photocatalytic Activity (V.Beena<sup>1</sup>, S. L. Rayar<sup>2</sup>, S.Ajitha<sup>1</sup>)
26. Synthesis and structural characterization of zinc doped magnesium oxide (B.C. Abhinisha<sup>(1)</sup>, T.R Jeena<sup>(2)</sup>)
27. XRD characterization of zinc oxide (ZnO) nano particles prepared by solution based method (<sup>1</sup>Abhirami.U.M; <sup>2\*</sup>Murugavel.S)

Potential Energy Distribution (PED) calculation. The hyperconjugative interaction which gives stability to the molecules has been analyzed using natural bond orbital (NBO) analysis. The charge transfer within the molecule and various molecular parameters such as ionisation potential, electron affinity, electronegativity, chemical potential, hardness, softness, and global electrophilicity index were determined using HOMO and LUMO analyses. Anti oxidant, antiviral and anti-inflammatory properties were revealed using molecular docking calculation.  
Keywords: Gaussian, HOMO, LUMO, docking, DFT.

**OP-17**

**Structural, computational, C-H...O/N-H...O hydrogen bonding, HOMO-LUMO, MESP and NBO analysis of N-2(hydroxy phenyl) acetamide**

**M.Jini pramila<sup>1</sup>, D.Arul Dhas<sup>2\*</sup>**

<sup>1</sup>Register number: 20213112132017, Research Scholar, Manonmanium Sundaranar University, Abishakapatti, Tirunelveli, Tamilnadu, India.

<sup>2\*</sup>Associate Professor, Department of physics and Research centre, Nesamony Memorial Christian College, Marthandam-629165, TamilNadu, India.

**Abstract**

Quantum chemical calculations of N-2(Hydroxy phenyl)acetamide(N2HPA) in the ground state was carried out by using density functional theory (DFT/B3LYP) method with 6-31G (d,p) basis set. The HOMO and LUMO energy levels are constructed and the corresponding frontier energy gaps are determined to realize the charge transfer within the molecule. The molecular electrostatic potential (MESP) and natural bond orbital (NBO) analysis have been used to evaluate the intermolecular interaction, especially the hydrogen bonds.

Keywords: - DFT, NBO, MESP.

**OP-18**

**Single crystal growth and optical properties of glutaric acid doped potassium hydrogen phthalate single crystals**

**A. Rathika<sup>a</sup>, R. Ganapathi Raman<sup>\*</sup>**

<sup>a</sup>Department of Physics and Research Centre, Muslim Arts College, Thiruvithancode, Thuckalay- 629 175, Tamilnadu, India, Affiliated to Manonmaniam Sundaranar University, Tirunelveli - 627 012

<sup>\*</sup>Department of Physics and Research Centre, Noorul Islam Centre for Higher Education, Kumaracoil- 629 180, Tamilnadu, India, Affiliated to Noorul Islam University, Kumaracoil- 627 175

<sup>a</sup>email:rathikarathi87@gmail.com

**Abstract**

Potassium hydrogen phthalate (KHP), a semiorganic material is one of the important NLO crystalline material. The single crystals of 2 wt% glutaric acid doped KHP crystal was synthesized and white coloured good optical quality single crystals were grown deionized water as solvent by slow evaporation solution growth technique at room temperature. From the single crystal XRD, the doped KHP crystal belongs to orthorhombic system. From the powder XRD data, the Bragg peaks with specific  $2\theta$  angles confirm the crystallinity of the material. The doped KHP crystal is active in the UV-Vis region and the band gap of the crystal is found to be 4.2 eV. The wide band gap of the