

## Dr. Anuj Kumar

Associate Professor, Department of Physics

### Education :

M.Sc.(Physics) from D.E.I., Agra, Ph.D. from Lucknow University.

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### Areas of research interest:

- Computational studies on Structure, vibrational spectra and properties of applicable molecules having potential medicinal, electronic, conducting and biodegradable applications using Ab initio methods specially Density Functional theory (DFT).
- Synthesis and Characterization of nanoparticles and their use in energy storage devices.

### Brief Background

Dr. Anuj Kumar did his graduation and post graduation from D.E.I. Agra. He obtained his Ph.D. Degree from Lucknow University, Lucknow in the area of normal modes and spectroscopic studies of polymers. He excelled during his education. He was awarded Director's medal for securing highest marks in B.Sc. (Hons.) Physics in the University. He has qualified at reputed national exams like GATE and CSIR-NET. He has around nineteen years of research and teaching experience at various Institutions. He has guided three students for Ph.D and one for M.Phil and few others are pursuing research under his supervision. He is the member of many scientific and educational societies like Material Research Society of India, Indian Science Congress etc. He is associated with many International and National journals of high repute like 'Polymer', 'Journal and Molecular Structure etc. (published by Elsevier) either as reviewer or editor. He has published around 25 research papers in SCI/Scopus indexed International/National journals. He has attended numerous National/International conferences in various capacities like **paper presenter, invited speaker, session chair etc.**



## Publications (Last Five Years)

### National/International Journals

1. Mukta Tripathi and **Anuj Kumar**, Synthesis and electrical studies of nano-composite polymer gel electrolyte for application in Supercapacitors, Material Science and Engineering:B, under review. [**Impact Factor: 3.316, Elsevier (SCI)**]
2. Mukta Tripathi, Santosh Bobade and **Anuj Kumar\***, Preparation of Polyvinylidene fluoride co-hexafluoropropylene based Polymer Gel Electrolyte and its performance evaluation for application in EDLCs, Bulletin of Materials Science, Accepted. [**Impact Factor: 0.925, Springer (SCI)**]
3. Mukta Tripathi and **Anuj Kumar\***, Zinc oxide nanofiller-based composite polymer gel electrolyte for application in EDLCs, Ionics (2018) 24:3155-316 [**Impact Factor: 2.347, Springer (SCI)**]
4. Mukta Tripathi and **Anuj Kumar\***, Electrochemical studies of EDLC Cells fabricated using drum stick (DS) activated charcoal, Materials Today: Proceedings 5 (2018) 15458–15465 [**Impact Factor: New, Elsevier (Scopus)**]
5. Mahendra Singh Yadav, Narendra Singh, **Anuj Kumar**, Synthesis and characterization of zinc oxide nanoparticles and activated charcoal based nanocomposite for supercapacitor electrode application, J Mater Sci: Mater Electron (2018) 29: 6853. [**Impact Factor: 2.324, Springer (SCI)**]
6. Mahesh Pal, Singh Yadav and Anuj Kumar\*, Theoretical investigations on NLO crystal 1-[4-(methylsulfanyl) phenyl]-3-(4-nitrophenyl) prop-2-en-1-one, *Asian Journal of Physics* Vol. 27 No 1, 2018, 23-34. [SSN:0971-3093]
7. Mahendra Singh Yadav, Narendra Singh, and **Anuj Kumar\***, ZnO Nanoparticles-Activated Charcoal Nanocomposite Electrodes for Supercapacitor, Adv. Sci. Eng. Med. 10, 659–664 (2018).[EMBASE (Elsevier)]
8. **Anuj Kumar\*** and Mahesh Pal Singh Yadav, Computational studies of third-order nonlinear optical properties of Pyridine derivative 2-Aminopyridinium p-Toluenesulfonate crystal, *Pramana*, 89(1), 2017; 39-45. [**Impact Factor: 0.692, Springer (SCI)**]
9. Mahesh Pal Singh Yadav and **Anuj Kumar\***, Quantum Chemical Computation by DFT Application of NLO Molecule 2-Aminopyridinium p-Toluenesulfonate. *Pramana*, 89(1),2017; 101-113. DOI 10.1007/s12043-017-1407-y. [**Impact Factor: 0.692, Springer (SCI)**]
10. Mahesh Pal Singh Yadav and **Anuj Kumar\***, A. Jayarama, “Vibrational spectra analysis, NBO, HOMO–LUMO, and nonlinear optical behavior studies on 3-(3,4-dimethoxyphenyl)-1-(pyridin-2-yl)prop-2-en-1-one”, *Monatshefte für Chemie - Chemical Monthly*, 147:1045–1061, 2016.[**Impact Factor: 1.222, Springer (SCI)**]

11. **Anuj Kumar\*** and Ravi Kant Upadhyay, “Optical, structural and morphological studies of ZnS nanoparticles synthesized using inorganic capping agent”, *J Mater Sci: Mater Electron* (Springer), volume 26, pp. 2430–2435, 2015. [**Impact Factor: 1.966, Springer (SCI)**]
12. **Anuj Kumar\***, Sapna Pathak and Poonam Tandon, “Molecular structure, vibrational spectra and nonlinear behavior of L-Lysine Monohydrochloride Dihydrate Crystal”, *JUET Research Journal of Science & Technology*, Volume 2, Issue 2, p.p. 169-191, 2015. (ISSN **2321-6026**)
13. Mahesh Pal Singh Yadav and **Anuj Kumar\***, “Molecular Structure and Vibrational Analysis of 2-Amino- 5-(m-Nitrophenyl)-1,3,4-Thiadiazole by DFT Calculations”, *International Journal of Materials and Chemistry*, Volume 4, Issue 3, pp 51-64, 2014. [**Scientific & Academic Publishing ( EBSCO A-to-Z)**] (e-ISSN: 2166-5354)

#### **FUNDED RESEARCH PROJECT COMPLETED:**

Title: Synthesis of nanomaterials using chemical approaches and their possible application in water purification.

Funding Agency: Madhya Pradesh Council of Science and Technology

Duration : 2 yrs. ( July 01, 2012 to June 30, 2014)

#### **Conferences (National/International) (Last Five Years)**

1. **Anuj Kumar**, “Density Functional Theory: An application to Molecular structure, vibrational spectra and electronic properties studies of a nonlinear crystal”, Invited talk delivered at 10<sup>th</sup> National Conference on Solid State Chemistry & Allied Areas, Delhi Technological University, Delhi , 1-3 July 2017
2. **Anuj Kumar**, “Investigations on Vibrational spectra, NBO and HOMO-LUMO of chalcone crystal 1-[4-(methylsulfanyl) phenyl]-3-(4-nitrophenyl) prop-2-en-1-one - A computational approach”, Invited talk delivered at 6<sup>th</sup> International Conference on Perspectives in Vibrational Spectroscopy, 5-8, November, 2016, Lucknow, India
3. **Anuj kumar** and Mahesh Pal Singh Yadav, “Computational studies of third-order nonlinear optical properties of Pyridine derivative 2-Aminopyridinium p-Toluenesulfonate crystal”, International E-Workshop/Conference on Computational Condensed Matter Physics and Materials Science" IWCCMP-2015 organised by ABV-IIITM, Gwalior , pp, ISBN, 18-22 October. 2015.
4. Mahesh Pal Singh Yadav and **Anuj kumar**, “Ab-initio investigations on NLO crystal 1-[4-(methylsulfanyl) phenyl]-3-(4-nitrophenyl) prop-2-en-1-one”, International E-Workshop/Conference on Computational Condensed Matter Physics and Materials Science" IWCCMP-2015 organised by ABV-IIITM, Gwalior , pp, ISBN, 18-22 October. 2015.
5. Mahesh Pal Singh Yadav and **Anuj kumar**, “Quantum Chemical Computation By DFT Application Of NLO Molecule 2-Aminopyridinium p-Toluenesulfonate”,

International E-Workshop/Conference on Computational Condensed Matter Physics and Materials Science" IWCCMP-2014 organised by ABV-IITM, Gwalior , pp, ISBN, 25-30 Nov. 2014.

6. **Anuj Kumar** and Mahesh Pal Singh Yadav , “Quantum Chemical Studies for Pharmacologically Significant Thiadiazole Derivative., International Symposium on Advances in Biological & Material Sciences, Lucknow University, 15 July 2014.
7. **Anuj Kumar**, Mahesh Pal Singh Yadav & Poonam tandon, “Density functional theory application on molecular structure and vibrational spectra studies on 2-amino-5-(m-nitrophenyl)-1,3,4-thiadiazole ” ,Fourth international conference on perspectives in vibrational spectroscopy (ICOPVS-2013), Bishop Moore College, Mavelikara, Kerala, 6-9, August, 2013