Curriculum-vitae

Personal Information-

Name-	Dr. Anoop Kumar Pandey
Designation-	Working as Assistant Professor Physics,K.S.Saket P.G.College AyodhyaFaizabad from 30/04/2019
Gender-	Male
Marital Status-	Married
Nationality-	Indian
Present address:-	Assistant Professor department of Physics, Kamata Prasad Sundal lal P.G.College Ayodhya.Uttar Pradesh,India-224123
Permanent Address-	Village- Sekhauliya, PO- Annapur, District- Ambedakar Nager, UttarPradesh, India, Pin Code- 224181

E-mail- anooppandeyias@gmail.com

Academic Qualifications:

Course	Board/University/Institute	Division	% of Mark
High School	U.P. Board Allahabad	1st	70.60
Intermediate	U.P. Board Allahabad	1st	65.2
B.Sc.	University, R.M.L.Avadh Faizabad	1st	66.08
M.Sc (Physics)	University, R.M.L.Avadh Faizabad	1st	68.50
Ph. D. (Physics *)*	*Lucknow* University		
NET-JRF	**UGC/CSIR**	2004	
GATE	**IIT/IISC**	2007(AIR310th)2008(AIR 82th)	

Training/Orientation/Refresher Coerces-

1. Orientation Course Conducted by ASC, Lucknow University Dated- 21Sep – 20 Oct. 2015.
2. Refresher Course on environmental science (Interdisciplinary) conducted by Human Resource Development Centre, GGU University, Bilaspur. Dated- 1Sep to 23 September,2016.
3. FDP Program on Advanced concepts for developing MOOCSconducted by Teaching Learning center Ramanujam College University of Delhi sponsored by MHRD Pandit Madan Mohan Malveeya National Mission on teachers and teaching Dated- 2july to 17 July 2020
4. FDP program on Badalata Bharteey Pridrishya:Sahitya Sanskrit Sanchar aur Manovigyan conducted by Ramanujam College University of Delhi sponsored by MHRD Pandit Madan Mohan Malveeya National Mission on teachers and teaching Dated 22-28 May 2020
5. FDP program on Sahitya Media monovigyan aur Vanijya ke vividh aayam conducted by Ramanujam College University of Delhi sponsored by MHRD Pandit Madan Mohan Malveeya National Mission on teachers and teaching Dated 29 May to 03 June 2020

Membership of Professional/Learning Bodies:

1. Former Member of editorial board of Scientific research and advances
2. Member of editorial board of **TMU Journal of Basic and Applied Chemistry**
3. Former Member of Board of studied of Bastar University Jagadalpur
4. Member of New BSc Physics Syllabus designing committee C.G. 2018-19

Teaching Experience-

Teaching in UG and PG classes from 30.04.2019 in K S Saket P G College Ayodhya U P to till now

Teaching in UG and PG Classes, from – 28/08/2017 to 29/04/2019 as Assistant Professor(Physics) in Govt.College Bishrampur

Teaching in UG and PG Classes, Joining Date- 27/11/2012 to 26/08/2017 as AssistantProfessor (Physics) in Govt. Danteshwari PG College Dantewada (CG)

Teaching experience of UG classes of engineering physics Joining date 10/02/2011 to28/02/2012 in SITM Lucknow.

Teaching in UG and PG Classes, Joining Date- 15/07/2005-28/02/2006 as Lecturerb(Physics) in Ganpat Sahay P.G. College Sultanpur (UP)

Administrative work-

1. Worked as Chairman of UGC Coordinator in Govt. Danteshwari PG College Dantewada Districtnodal of New Education Polity of India in Dantewada
2. Different college level responsibilities like- Assistant superintendent in exams, discipline, sports, cultural and other co-curricular committees
3. Former HOD of Physics, in Govt. Danteshwari PG College Dantewada
4. Former Member of RUSA, IQAC and other committees in our college
5. Member of designing new curriculum for Physics in UG level course of Chhattisgarh.

Ph.D Research

Title of thesis: Study of Vibrational modes analysis geometry optimization ,single point energy of some macromolecule by using Ab-initio technique

My Ph.D research has involved the theoretical investigation of molecular structure, vibrational spectra, thermodynamic and potential energy distributions of bioactive Macromolecules andNano-Clusters, using quantum chemical methods. I have performed quantum chemicalcalculations using ab initio Hartree-Fock and Density Functional Theory (DFT) methods, making use of the Gaussian 03W program; these included geometry optimization and calculation of harmonic frequencies, entropy, total energy and other thermodynamic properties. More specifically, I studied in detail these properties for 2-formyl benzonitrile,Cyclobuteonecyclobutnone,Loganin,III-Vgroup clusters, Diboried clusters,C60 clusters doped with trasition metal. All of these compounds are of great pharmaceutical importance. I compared these results with experimental FT-IR and FT-Raman spectra, obtaining excellent agreement, which served to validate the computational techniques. I also compared calculated structural parameters with available crystallographic data, again showing excellent agreement. I also calculated normal mode vibrational frequencies, and used the principles of statistical mechanics to relate these to thecomputed and observed thermodynamic properties. My Ph.D. research work also involved comparative vibrational studies of two well-known organic compound cyclobuteone and cyclobutnone. I analysed the similarities and differences between the vibrational spectra of these molecules, which helped to interpret the X-ray structure and infrared spectra of these natural products. I have recently finished calculations of thermodynamic properties of these biomoleculesto rationalise their observed macroscopic behaviour.

In addition to work on my Ph.D thesis, I also have working experience of molecular mechanics (MM) methods, using Urey-Bradley force fields (UBFF). In addition to valence force fields, these account for non-bonded interactions in the *gem* and *cis* configuration, and for tension terms. I have found that the MM approach gives a better description of intra- and inter-unit interactions, and it reduces the somewhat arbitrary nature of choosing the force constant. I have also performed hybrid QM/MM calculations, using the ONIOM approach in Gaussian, to optimizationof the molecular structure, boldine hydrochloride. I found that the geometry and vibrational spectra obtained by this hybrid approach were very accurate. This shows that QM/MM methods will be vital to lead to more rapid treatment of larger macromolecules, in place of time- consuming ab initio methods, and I seek to refine and develop my expertise in this area.

Scientific skill

- Quantum Mechanics based research work. Knowledge of Molecular Mechanics, Semi empirical, Ab initio, Density Functional Theory and QM/MM methods.

Computational skill

- Working Experience in different interface
- Programming with FORTRAN, and Assembly Language
- Knowledge of Computer maintenance

Scientific computational skill

- Working experience in Gaussian 16, AMBER, Argus lab, Hyper Chem, GAMESS(US) and VEDA software's, Origin 8.0 software, Chemcraft, Gauss Sum

Personel Details

Father's Name	:	Shree Ram Pandey
Date of Birth	:	28-feb-1981
Marital Status	:	Single
Nationality	:	Indian

Languages

English
Hindi

References

Prof. Neeraj Misra
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University of Lucknow, Lucknow- 226007, India
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Email: neerajmisra66@gmail.com
Prof. Onkar Prasad
Department of Physics
University of Lucknow, Lucknow-226007, India
Cell Phone No. +91-9415001434
Email: onkarprasad1@gmail.com

- **Research Activities:**

Organizing Conference/Seminar/Workshop

1. **Organizer of "Workshop on Bio-diversity Conservation"**. Organized by Govt. Danteshwari PG College Dantewada (CG) and funded by Ministry of Environment and Forest, Government of India via Jan Kalyan Parishad. Dated- 13 February, 2014.

2. **Member of Organizing** committees **"**National Seminar on Challenges of Human Resource Development in Tribal Areas". In Govt. Danteshwari PG College Dantewada (CG). Dated- 16-17 January, 2015.

Projects Online

One Ongoing Mini Research project founded by U P Government entitled **"Molecular Docking DFT calculation of some important biologically active molecule and their interaction with metal " of amount three lakhs rupees of three years**

Research guidance

- Two students enrolled avinash kumar Mishra and ankit kumar sharma for PhD in Dr R M L Avadh University Ayodhya
- Guidance of 13 student for submission Project in Physics in Bastar University Jagadal pur .

List of Published and Communicated Books

- A handbook of engineering Physics Vol.-I lulu publication 2018 ISBN: 978035918639
- A handbook of engineering Physics Vol.-II lulu publication 2018 ISBN: 978035918639
- An Introduction to Thermodynamics and Statistical Physics
- INNOVATIVEPUBLICATIONBOOKS 2021 ISBN: 978-93-88022-74-3
- Concept of Physics and its Application P K publisher and distributor ISBN:978-93-92239-16-8
- Text Book of 11-12 for Bihar Jharkhand Board BMD publication (communicated)

LIST OF PUBLISHED PAPERS

During 2007-2012

- Electronic Structure, Optical Properties and Vibrational Analysisof2-Decenoic acid and its derivative by Density Functional Theory,ApoorvaDwivedi, **AnoopKumar Pandey**, NeerajMisra. , Spectroscopy 26 (2011) 367–385.
- FTIR spectra and Vibrational Spectroscopy of Loganin using Density Functional Theory, **AnoopPandey**, Shamoon A Siddiqui, ApoorvaDwivedi, NeerajMisra, Kanwal Raj, Spectroscopy 25 (2011) 287–302.
- Quantum chemical study of RhF_nnano clusters: An investigation of superhalogen propertiesShamoon Ahmad Siddiqui **Anoop Kumar Pandey,**TabishRasheedMahima Mishra in Journal of Fluorine Chemistry Volume 135, March 2012, Pages 285–291.
- Vibrational analysis of boldine hydrochloride using QM/MM approach NeerajMisra, Shamoon Ahmad Siddiqui, Ruby Srivastava,**Anoop Kumar Pandey**Sudha Jain,.*Spectroscopy Vol. 24 No. 5, (2010) 483-499.*
- Molecular structure and vibrational spectra of 2 formylbenzonitrile by dendity functional theory and ab-initio Hartree-Fock calculations", NeerajMisra, Onkar Prasad, LeenaSinha, **AnoopPandey,**Journal *of Molecular Structure: THEOCHEM 822 (2007) 45-47.*
- Molecular structure, vibrational spectra and potential energy distribution of colchicine using ab initio and density functional theory", Shamoon Ahmad Siddiqui, **Anoop Pandey**, P. K. Singh, TanveerHasan, Sudha Jain, NeerajMisra,*Journal of Computer Chemistry, Japan Vol. 8, No. 2 (2009) 59-72.*
- Semi-empirical Studies of different structures of fullerene rings Doped with Transition metals, ApoorvaDwivedi, **Anoop Kumar Pandey**, Onkar Prasad, LeenaSinha, NeerajMisra. *Chinese Journal of Physics*,CHINESE JOURNAL OF PHYSICS VOL. 50, NO. 1 2012.
- Structural, Vibrational and Electronic properties of ring structures of small ZrO clusters in lower and higher spin state- A DFT Study,NeerajMisra, ApoorvaDwivedi, **Anoop Kumar Pandey**, Journal of Atomic Molecular Science. Vol. **3**,No. 3, pp. 187-196 2012.
- Electronic structure, non linear optical properties and vibrational analysis of gemifloxacin by density functional theory Shamoon Ahmad Siddiqui, TabishRasheed, Mohd Faisal, **Anoop Kumar Pandey**, SherBahadar KhanSpectroscopy: An International Journal Volume 27 (2012), Issue 3, Pages 185-206 doi:10.1155/2012/614710**.**
- Ab initio study of the endohedral fullerene PbH4@C60" Fullerenes, Nanotubes and Carbon Nanostructures**Anoop Kumar Pandey**, ApoorvaDwivedi 2012 22: 679–686, 2014 Taylor & Francis Group ISNN-1536-383X**.**
- Quantum chemical study of pure and transition metal (Ni, Pd, Pt) doped hydrogenated silicon nano cages, NeerajMisra, ApoorvaDwivedi, **Anoop Kumar Pandey**, J. Comput. Method. Mol. Design, 2011, 1 (2):22-33.
- Structural, Vibrational and Electronic properties of Ga_xS_y (x+y=2-5) nanoclusters- A DFT Study, ApoorvaDwivedi, **Anoop Kumar Pandey**, Neerajmisra, ***J. Comput. Method Mol. Design***2012, 2 (2):68-75.

- Quantum Chemical study and the effect of substitution of a Amino group on the reactivity of 4, Aminopyridine and 3,4 Diaminopyridine by Density Functional Theory", ApoorvaDwivedi, Shamoon Ahmad Siddiqui, **Anoop Kumar Pandey,**Onkar Prasad, LeenaSinha, NeerajMisra,*Der Pharma Chemica*, 2009, 1(2): 258-268**.**

- Comparative vibrational spectroscopic study of benzonitrile derivatives using density functional calculation, Neerajmisra, Shamoon A. Siddiqui, **Anoop Kumar Pandey**, SanjeevTrivedi, Der Pharma Chemica, 2009, 1 (1), 196-209.

- Comparative conformational, structural and vibrational study on the molecular structure of tyrosine and L-DOPA using density functional theory, Shamoon Ahmad Siddiqui, **Anoop Kumar Pandey**, ApoorvaDwivedi, Sudha Jain,NeerajMisra, *J. Chem. Pharm. Res.,* 2010, 2(4):835-850.

- Vibrational spectra and assignment of 3-(2-Nitrophenoxy) phthalonitrile by Ab initio Hartree-Fock and Density Functional Methods", Neeraj Misra, **AnoopPandey**,ApoorvaDwivedi, SanjeevTrivedi, Shamoon Ahmad Siddiqui, *Der Pharma Chemica,*2010, 2(4): 342-360.

- Study of Hafnium Diboride Clusters Using Density Functional Theory", NeerajMisra*, ApoorvaDwivedi, Onkar Prasad, **Anoop Kumar Pandey**, Archives of Physics Research, 2010, 1 (2): 15-19. [ISSN 0976-0970

- Vibrational analysis of Two Narcotic Compounds- Codeine and Morphine -A comparative DFT study,NeerajMisra, ApoorvaDwivedi, **Anoop Kumar Pandey**, SanjeevTrivedi,Der PharmaChemica, 2011, 3(3):427-448

- Comparative Study of Vibrational spectra of two well known natural products Lupeol and Lupenone Using Density Functional Theory,ApoorvaDwivedi, **Anoop kumar pandey**, Neeraj misra,***Spectroscopy***: An International JournalVolume 27(2012), Issue 3, Pages 155–166

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- Quantum chemical study of PtF_n and $PtCl_n$ (n=1-6) nano clusters: An investigation of superhalogen properties Shamoon Ahmad Siddiqui and Tabish Rasheed Anoop Pandey Computational and Theoretical Chemistry 979 (2012) 119–127.
- Quantum chemical study of RhF_n nano clusters: An investigation of superhalogen properties Shamoon Ahmad Siddiqui **Anoop Kumar Pandey,**Tabish Rasheed Mahima Mishra in Journal of Fluorine Chemistry Volume 135, March 2012, Pages 285–291.
- Semi-empirical Studies of different structures of fullerene rings Doped with Transition metals, Apoorva Dwivedi, **AnoopKumar Pandey**, Onkar Prasad, Leena Sinha, Neeraj Misra. *Chinese Journal of Physics*, CHINESE JOURNAL OF PHYSICS VOL. 50, NO. 1 2012
- Comparative study of vibrational spectra of two narcotic compounds using Density Functional Theory, **Anoop Kumar Pandey**, Shamoon Ahmad Siddiqui, NeerajMisra. *Chinese Journal of Physics*VOL. 51, NO. 3,2013.
- Structural, Vibrational and Electronic properties of ring structures of small ZrO clusters inlower and higher spin state- A DFT Study, Neeraj Misra, Apoorva Dwivedi, **Anoop KumarPandey**, Journal of Atomic Molecular Science. Vol. **3**,No. 3, pp. 187-196 2012.
- Electronic structure, non linear optical properties and vibrational analysis of gemifloxacin by density functional theory Shamoon Ahmad Siddiqui, TabishRasheed, Mohd Faisal, **Anoop Kumar Pandey**, SherBahadar KhanSpectroscopy: An International Journal Volume 27 (2012), Issue 3, Pages 185-206 doi:10.1155/2012/614710**.**
- Ab initio study of the endohedral fullerene PbH4@C60" Fullerenes, Nanotubes and Carbon

NanostructuresAnoop Kumar Pandey, ApoorvaDwivedi 2012 22: 679–686, 2014 Taylor & Francis Group ISNN-1536-383X.

- A combined experimental and quantum chemical studies on molecular structure, spectral properties, intra and intermolecular interactions and first hyperpolarizability of 4– (Benzyloxy)benzaldehydethiosemicarbazone and its dimer, Amit Kumar, PoonamRawat VikasBaboo, DivyaVerma, R.N. Singh, DeeptiSaxena, H.M. Gauniyal, **Anoop Kumar Pandey**, Harish Pal, *Journal of Molecular Structure*, *Volume 1034*, *27 February2013*, *Pages 374-385*
- Theoretical study of structural, vibrational, and electronic properties of Aluminiumantimonide, Gallium antimonide and Indium antimonide clusters, (AlSb, InSb, GaSb) n (n=1, 2, 3), **ANOOP PANDEY** et al, *J. Theor. Comput. Chem.* **12**, 1350056 (2013)
- Quantum Mechanical Study on the Structure and Vibrational Spectra of Cyclobutanone and 1,2-Cyclobutanedione,**Anoop Kumar Pandey**, ApoorvaDwivedi, Neerajmisra, Spectroscopy, Volume 2013 (2013), Article ID 937915, 11 pages. .
- Normal modes, Molecular Orbitals and Thermochemical analyses of 2, 4 anad 3, 4 dichloro substituted phenyl-N-(1, 3- thiazol-2-yl)acetamides: DFT Study and FTIR spectra," by Ambrish Srivastava, **Anoop kumarPandey**, BadiadkaNarayana, Balladka K. Sarojini and NeerajMisra. Journal of Theoretical ChemistryVolume 2014, Article ID 125841, 10 pages ISNN 1082-4928.
- Structural, Electronic, and Vibrational Properties of Isoniazid and Its DerivativeN- Cyclopentylidenepyridine-4- carbohydrazide: A Quantum Chemical Study Journal ofTheoretical ChemistryVolume 2014, Article ID 894175, 15 pagesISNN 1082-492
- Reactive nature, substitution reaction, structural and vibrational properties of 2, 3 Dichloropridine by DFT Study, Abhishek Bajpai, **Anoop Kumar Pandey**, Kamal Pandey, ApoorvaDwivediJournal of Computational Methods in Molecular Design, 2014, 4 (1):64- 69.
- Structural, Vibrational and Electronic properties of Ga_xS_y (x+y=2-5) nanoclusters- A DFT Study, ApoorvaDwivedi, **Anoop Kumar Pandey**, Neeraj misra, ***J. Comput. Method Mol. Design***2012, 2 (2):68-75.
- Comparative Study of Vibrational spectra of two well known natural products Lupeol and Lupenone Using Density Functional Theory,ApoorvaDwivedi, **Anoopkumarpandey**, Neerajmisra,***Spectroscopy***: An International JournalVolume 27(2012), Issue 3, Pages 155–166
- DFT Study of Picric acid and its derivative by first principles "Vijaynarayan, ApoorvaDwivedi, Abhishekbajpai, subodhpandey, **Anoop Kumar Pandey**, International Journal of Engineering Trends and Technology, Dec 2013 volume 4 issue 12. ISSN: 2231-5381.

- DFT Study Of Mndiboride(MnB2)N{N=1-3),**Anoop KumarPandey**,International Journal of Engineering Research and Technology(IJERT),December- 2013 ,Vol. 2 , Issue 12 issue,ISSN: 2278-0181**.**
- Structural, Electronic and Vibrational properties of Isoniazid and its derivative N- Cyclopentylidenepyridine-4- carbohydrazide-A quantum Chemical study, **Anoop Kumar Pandey**, VIkasBaboo, ApoorvaDwivedi, Hindawi Publishing Corporation Journal of theoretical Chemistry, Volume 2014, Article ID 894175, 15 pages.ISSN: 2314-6184.
- Reactive nature, substitution reaction, structural and vibrational properties of 2, 3 Dichloropridine by DFT Study, AbhishekBajpai,**Anoop Kumar Pandey**, Kamal Pandey, Apoorva Dwivedi, Journal of Computational Methods in Molecular Design.Page No: 64- 69, 2014,ISSN:2231-3176.
- Isolation, Identification**,** Molecular and Electronic Structure, Vibrational Spectroscopic Investigation and Anti-HIV-1 activity of Karanjin Using Density Functional Theory,**Anoop Kumar Pandey**, Abhishek Kumar Bajpai, Ashok Kumar, Mahesh Pal, VikasBaboo, ApoorvaDwivedi,Hindawi Publishing Corporation,Journal of theoretical Chemistry, 2014. ISSN: 2314-6184.
- Comparative Study of structural, vibrational, electronic properties of pentanoic acid (Valeric acid) and its derivative 4-oxopentanoic acid (Levulinic acid) by Density Functional Theory, "Abhishek Bajpai", Apoorva Dwivedi, **Anoop Kumar Pandey**,J. Sci. Res. Adv. 2014, 1(1), 18–24**.**
- Quantum chemical calculations of a novel Specie–Boron Nano Bucket (B16) and the interaction of its complex (B15-Li) with drug Resorcinol Pandey, Anoop Kumar; Singh, Vijay; Dwivedi, Apoorva Journal of Computational Methods in Sciences and Engineering 20 (2020) 1017–1028 1017 DOI 10.3233/JCM-200032
- Vibrational and Structural Properties of Ethyl (1RS,6SR)-4- (2-methyl-1H-imidazol-4-yl)-2-oxo-6-(2,3,5-trichlorophenyl)- cyclohex-3-ene-1-carboxylate by DFT Abhishek Khare1 , Amarendra Kumar1 , Atul Tiwari2 , Anoop K. Pandey3 and Vijay Narayan4 Journal of Chemistry and Chemical Sciences, Vol.7(10), 802-811, October 2017
- Electronic Vibrational and Structural Properties of Methyl Picolinonitrile, 1-oxide by DFT Abhishek Khare, Amarendra Kumar, Atul Tiwari, Anoop K. Pandey and Vijay Narayan Journal of Chemistry and Chemical Sciences, Vol.7(10), 793- 801, October 2017
- Structure, Biological activity, IR UV spectra of sulfur derivative of pyrazine using DFT method Atul Tiwari, 2 Anoop Kumar Pandey International Journal of Zoology Studies Volume 3; Issue 1; January 2018; Page No. 112-117 Chemical and biological activity of login: A DFT study Atul Tiwari, 2 Anoop Kumar Pandey International Journal of Zoology Studies Volume 3; Issue 1; January 2018; Page No. 118-122
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- Geometry optimization, Electronic Properties, UV spectra and NLO analysis of 5- nitro- picolinamide by using First principle Anoop Kumar Pandey, Vinod Kumar Singh , Gaurav Mishra , Vijay Singh TMU Journal of Basic & Applied Chemistry Vol.1 Jan-December, 2021:pp. 13-21
- Molecular modeling and vibrational properties of 5-Bromobenzene-1, 3-dicarbonitrile using Density Functional Theory,Abhishek Kumar Bajpai, Manisha Singh, AnjuYadav, **Anoop Kumar Pandey** and Apoorva Dwivedi,J. Sci. Res.Adv. 2014, 1(1), 03–07.
- Normal modes, molecular orbitals and thermochemical analyses of 2, 4 and 3, 4 dichloro substituted phenyl-N-(1, 3- thiazol-2-yl)acetamides: DFT study and FTIR spectra Published J. Theoretical Chem. 2014**.**
- Uniform versus non-uniform scaling of vibrational bands: A test on 2-(2,6- Dichlorophenyl)-N-(1,3-thiazol-2yl) acetamide, Ambrish Srivastava, **Anoop Kumar Pandey,** Neeraj Mishra**,** Published Int. J. Spectroscopy, 2014.
- FT-IR spectroscopy, intra-molecular C-H···O interactions, HOMO, LUMO, MESP analyses and biological activity of two natural products, Triclisine and Rufescine: DFT and QTAIM approaches, Ambrish Srivastava, **Anoop Kumar Pandey,** Neeraj Mishra Spectrochim. ActaA Vol-136,682-689 (2015)**.**
- Quantum chemical and spectroscopic investigations on cis and transconformers of 4- hydroxy-l-proline, Ambrish Srivastava, **Anoop Kumar Pandey,** Neeraj Mishra J. At. Mol. Sci. Vol. 5, No. 4, pp. 279-288 November 2014**.**
- Study of small Niboium Sulphide cluster NbmSn(n,m=1-2) Saurabh kumar Ambrish kumar srivastva Anoop Kumar Pandey Neeraj Mishra J.At.Molecular sciences September 2014The Journal of Atomic and

Molecular Sciences 5(3):231-237

- Stability and electronic properties of transition metal antimonides in ionic and neutral case-TMmSbn(m, n=1- 2)Abhishek Kumar Bajpai, Apoorva Dwivedi and Anoop Kumar Pandey Page No: 38-45, 2014 JCMMD .
- Quantum chemical study on2-bromo-3- hydroxy-6-methyl pyridine-A D. F. T. study Apoorva Dwivedi and Anoop Kumar etal.Page No:411-417,2014, JCPOR.
- Quantum chemical study on 2, 6 Bis (Bromo-methyl) Pyridine- A D.F.T Study. Apoorva Dwivedi, Anoop KumarPandey and Abhishek Bajpai, Der Pharma Chemica, 2014.
- Superconducting properties of Zinc Diboride Nanoclusters Apoorva Dwivedi, Anoop Kumar Pandey and AbhishekBajpai, *J. Sci. Res. Adv. Vol. 2, No. 1, 2015, 48-50.*
- Structural, electronic and vibrational study of the endohedral fullereneSiH4@C60 Ab initio study Apoorva Dwivedi, Anoop Kumar Pandey and Abhishek Bajpai,*Cite this article: J. Sci. Res. Adv. Vol. 2,* 5 *No. 2, 2015, 69-72*
- Ab-initio study of 'N'-hydroxy-pyrimidine2carboximidamide by Density Functional Theory Apoorva Dwivedi, AnoopKumar Pandey and Rashmi Devangan, *J. Sci. Res. Adv. Vol. 2, No. 4, 2015, 158-162.*
- A quantum chemical study of YFn nano clusters – An investigation of superhalogen properties Anoop Kumar Pandeya,Ambrish Kumar Srivastava and Apoorva Dwivedi Main Group Chemistry 14 (2015) 291–299
- Structural, Electronic Properties, Hydrogen Bonding Analyses, and Biological Activity of Two Multiple Myeloma Drugs: Lenalidomide and Pomalidomide Ambrish Kumar Srivastava Anoop Kumar Pandey Saurabh Pandey Polycyclic Aromatic Compounds Volume 36, 2016 - Issue 4
- Quantum Chemical Study on 5-(1,3-Dithian-2-Y L)- 2H-1,3-Benzodioxole- AD.F.T Study Abhishek Bajpai1 , VinodDubey2 , V. K. Singh3 , A. K. Singh4 , Vijay Narayan Mishra5*, Kamal Kumar Pandey6 and Anoop Kumar Pandey Journal of Chemistry and Chemical Sciences, *Vol.6(1), 78-87, January 2016*
- Vibrational analysis of 1-Methyl-3-phenylthiourea- A density functional theory basedstudy Apoorva diwedi,Rupa yadavAnoop Kumar Pandey, *J. Sci. Res. Adv. Vol. 2, No. 3, 2015, 131-135*
- Quantum chemical investigation on structures and energetics of Tungsten Fluoride (WFqn) species (q = 0, ±1; n < 6) Ambrish K Srivastva,Anoop Kumar Pandey Neeraj Mishra *J. Chem. Sci.* Vol. 127, No. 10, October 2015, pp. 1853–185
- *Ab-initio* study of '2-(3-bromo phenyl)1,3-dithian by density functional the Abhishek Bajpai1 , Anoop Kumar Pandey2and Vijay Narayan Mishra ory Journal of Chemical and Pharmaceutical Research, 2016, 8(1):675-681
- Quantum chemical origin of high ionization potential and low electron affinity of Tungsten Hexafluoride Ambrish Kumar Srivastava, Anoop Kumar Pandey2 and Neeraj Misra1 Journal of Computational Methods in Molecular Design,2015, 5 (4):142-146
- Quantum chemical study of 4-chloro-3-ethylphenol Apoorva Dwivedi, Anoop Kumar Pandey,Vinod dubey, AbhishekBajpai,*J. Sci. Res. Adv. Vol. 2, No. 1, 2015, 38-41*
- Correction: The biological activity and molecular docking studies of three multiple myeloma drugs Ambrish KumarSrivastava Anoop Kumar Pandey Apoorva diwedi, Ravish Das J. Sci. Res. Adv. Vol. 2, No. 2, 2015, 101-101
- Quantum chemical study on 2,6-bis(bromo-methyl)pyridine-A D.F.T. study Apoorva Dwivedi1 , Anoop Kumar Pandey Der Pharma Chemica 7(1):55-61 2-152015
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- VIBRATIONAL ELECTRONIC NLO AND NBO STUDY OF 4-PYRAMIDINE NITRILE BY AB-INITIOMETHODGLOBAL JOURNAL OF MULTIDISCIPLINARY STUDIE Volume-5, Issue-9, August- 2016
- Comparative Study of structural, vibrational, electronic properties of pentanoic acid (Valeric acid) and its derivative 4-oxopentanoic acid (Levulinic acid) by Density Functional Theory J.Sci.res.Adv 2014 1(1) 18-24

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- Stability and electronic properties of transition metal antimonides in ionic and neutral case-TMmSbn(m, n=1- 2)Abhishek Kumar Bajpai, Apoorva Dwivedi and Anoop Kumar Pandey Page No: 38-45, 2014 JCMMD .

List of publication during 2017-2021

- Investigations on the frontier orbitals of FeFn (n = 1-6) superhalogen complexes and prediction of novel salt series Li ─ (FeFn) Journal of Fluorine Chemistry 195 (2017) 85– 92
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List of publication and Accepted papers during 2022-23

- Molecular docking, experimental FT-IR spectra, UV–Vis spectra, vibrational analysis, electronic properties, Fukui function analysis of a potential bioactive agent – Proflavine ,, O.P.Yadav[a] Apoorva Dwived Journal of the Indian Chemical Society Volume 99, Issue 4, April 2022, 100396 **(IF=0.24)Elsevier**
- Comprehensive quantum chemical calculations and molecular docking analysis of uracil mustard by first principle Journal of the Indian Chemical Society 202299(7):100580**(IF=0.24)Elsevier**
- Investigation of superacidic behavior of hydrogenated FemFn (m = 1/2,n = 1–6/11) complexes and their abilities to form supersalts Anoop Kumar Pandey · Apoorva Dwivedi· Dharmesh Vikram Shukla · Avinash Kumar Mishra Benard Samwel Mwankemwa · Vijay Singh Structural Chemistry https://doi.org/10.1007/s11224-022-02099-4 **(IF=2.012) Springer**
- Quantum Chemical Analysis and effect of super alkali/ super halogen doping on the opto-electronic properties of L-lysine p-nitrophenolatemonohydrate (LLPNP) using First principle", which you submitted to Polycyclic Aromatic Compounds, has been reviewed. Your work provides an extensive computational analysis of LLPNP (L-lysine pnitrophenolatemonohydrate) Anoop Kumar Pandey Vijay Singh, Apoorva diwedi Polycyclic aromatic compound 2022(accepted)**Taylor Francis (IF=3.774)**
- Time dependent density functional theory, AIM Analysis, NLO and Thermodynamic properties of Propofol and adsorption effects of Propofol drug over Carbon nanotube (C56H16) as the factor of drug delivery system *Macromol. Symp.* **2023**, *407*, 2100451
- Comparative Study of Molecular Docking, Structural, Electronic and Fukui Function studies on Favipiravir and its newly designed derivatives (Potential Inhibitors) for COVID-19 Protease *Macromol. Symp.* **2023**, *407*, 2200028 (IF=0.90)
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- Quantum chemical study of effect on adsorption properties of Antituberculosis drug N-Cyclopentylidenepyridine-4-carbohydrazide interaction with CNT(C56H16) Journal of the Indian Chemical Society Volume 100, Issue 1, January 2023, 100851 **(IF=0.24)**
- Influence of electric field on the electro-optical and electronic properties of 4-n-alkoxy-4′-cyanobiphenyl liquid crystal series: Anoop Kumar Pandey; Vijay Singh; Kamal Kumar Pandey; Apoorva Kumar Dwivedi; Madan Singh Chauhan; Dipendra Sharma An ab initio study Pramana - Journal of Physics *Pramana – J. Phys.* (2023) 97:93 IF=2.70)
- V N Mishra A K Pandey , A Dwivedi , B S Mwankemwa , AMaurya , A K Sharma , V Singh Comprehensive quantum chemical calculations and molecular docking analysis of uracil mustard by first principleJournal of the Indian Chemical Society 99 (2022) 100580
- A K Pandey∗, A K Sharma∗, S Shukla ,AMishra†, V Singh‡ and ADwivedi§Molecular docking, QTAIM analysis, UV-Vis spectra vibrational analysis, and electronic properties of Lantadenes C and D — A complete comparative studyInternational 1 Journal of Computational Materials 2 Science and Engineering (2023) 2350028 (28 pages)
- Stimulated Raman side and back scatter instabilityof crossed laser beam in plasma A K Pandey,V Singh High energy density physics (2023) xxx(xxxx)101054
- *A.K. PANDEY*, V.K. SINGH**, A.K. SHARMA*, S.N. TIWARI*, G. MISHRA*, R.K.S. YADAV V.N. MISHRA*SPECTROSCOPIC, NLO, NBO, BIOCHEMICAL INVESTIGATIONOF3-(HYDROXYMETHYL)-3-METHYL-2,6DIPHENYLPIPERIDIN-4-ONE ROMANIAN J. BIOPHYSICS(Accepted)
- Superacidic properties of protonated PtFn(n=1-6) and their ability to form supersalts: DFT study V Singh.D V Shukla,A Soni A K Pandey Macromolecule symposia 2023(Accepted)
- A quantum chemical study on the enormously large nonlinear optical response of doped endohedral superalkali Na2F and superhalogens MF4 (M=B, Al) with CNT(C56H16) cage

V Singh.A Diwedi A tiwarim A K Pandey Macromolecule symposium 2023(Accepted)

- Variation in structural chemical reactivity and nonlinear optical (NLO) properties ofStimulated $C_{56}H_{16}$ nanotube after endohedral doping of superalkali (Na_2F) and superhalogen (BF_4): A DFT study V Singh A Dwivedi, A K Mishra, A K Pandey Chemistry Africa 2023 (Accepted)

Paper published in Conference Proceeding

- ❖ Geometry Vibrational and NBO analysis of thiozole derivatives (Z)-4-{[4-(3-methyl-3-phenylcyclobutyl)thiazol-2-yl]amino}-4-oxobut-2-enoic acid Anoop Kumar Pandey, Ankit Kumar Sharma, V K Singh, Benard S. Mwankemwa, Vijay Singh in proceeding of International conference on emerging trends in IoT& Computing technologies -2022 paper presented entitled organized by G.I.T.M. along with G.I.P.S. Lucknow(U.P.) India associated with **CRC press (Taylor &Francis Group)** dated 13-14 May 2022.ISBN: 9781003350057 DOI:10.1201/9781003350057
- ❖ Quantum chemical study Thiozole derivatives cyclobutyl molecule C18H18N2O3SAnoop Kumar Pandey, Ankit Kumar Sharma,Avinash Mishra, Satyendra Nath Tiwari,Vijay Singh in proceeding of International conference on emerging trends in IoT& Computing technologies -2022 paper presented entitled organized by G.I .T.M. along with G.I.P.S. Lucknow(U.P.) India associated with **CRC press (Taylor &Francis Group)** dated 13-14 May 2022.ISBN: 9781003350057 DOI:10.1201/9781003350057
- ❖ The simulation stud of small signal CE amplifiers and Darington amplifier Satyendra Nath Tiwari, Gaurav Mishra, Anoop Kumar Pandey Shiv Kumar and Vijay Singhin proceeding of International conference on emerging trends in IoT& Computing technologies -2022 paper presented entitled organized by G.I .T.M. along with G.I.P.S. Lucknow(U.P.) India associated with **CRC press (Taylor &Francis Group)** dated 13-14 May 2022.ISBN: 9781003350057 DOI:10.1201/9781003350057

Paper present and invited talk in seminar

- 14 Paper Present different seminar and 10 invited talk

The above-mentioned details are true to the best of my knowledge.

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