Name: Dr. N V Suresh Kumar

Designation: Assistant Professor of Physics
Department: H&S Department
Mail I'd: sureshkumar_nv@vnrvjiet.in

Experience (in years): Teaching: 16 Research: 10

**1. Educational / Technical qualifications:**

| S.No | Level (UG / PG / Ph.D) | Year of passing | Specialization |
|---|---|---|---|
| 1. | Ph. D | 2013 | QM Methods based Molecular Modeling |
| 2 | MTech. | 2009 | Biotechnology |
| 4. | M.Sc. | 1997 | Physics |
| 4. | B.Sc. | 1995 | Mathematics, Physics, Chemistry |

**2. Teaching and Learning:**

2.1. Teaching Interests: Physics and molecular modelling
2.2. Novel Teaching & Learning Techniques adopted: WIT & WIL

**3. Co-curricular and Extra-Curricular Activities: Nil**

**4. Conference / Workshop / Seminar / Guest Lectures :**

4.1 Conducted:

- Organized a training program on digital tools to new faculty of H&S on 5th, 6th 10th, 18th and 28th May 2021.
- Coordinator of a Webinar on Multifunctional Materials, organized by CNST, H &S, VNRVJIET, on 15th – 16th July 2020.

4.2 Attended:

- Presented poster in the international conference on chemistry and allied sciences-2022 at Pingle Government college for women, Hanumakonda, Warangal on 25-27 August 2022.
- AICTE sponsored 5 day FDP on International Human Values from 31 May 2021 to 4 June 2021.
- AMPLE LMS 2 day workshop on 20th and 22nd January 2021.

**5. Academic Contribution and Research & Consultancy:**

5.1. Invited Lectures:

- Resource person in IEEE summer school in Nanotechnology-2022, held during 16 -19th November -2022, at VNRVJIET-Hyderabad.

- Resource person for 4th International Conference on Recent Advances in Mathematical Sciences and Applications (RAMSA-21) from 21st to 24th December, 2021 on Virtual Mode, conducted by GVP College of Engineering, Visakhapatnam.

- A seminar presentation on Computational and Experimental tools of research in materials science, 25th August 2021, conducted by H&S department, VNRVJIET.

- Resource person for AICTE sponsored 2 weeks STTP on "Design and Structural Evolution of Advanced Functional Materials Suitable for Engineering Applications" organized by Department of Electronics and Instrumentation Engineering and Centre for Nanoscience and Technology - VNRVJIET-Hyderabad, from 15 -20 February 2021 and 1 – 6 March 2021.

- Resource person of a Webinar on Multifunctional Materials, organized by CNST, H &S, on 15th – 16th July 2020.

- Density functional theory for prediction of structure and reactivity of newly synthesized peptides, International symposium on chemistry with computers", IIIT-Hyderabad, IICT - Hyderabad, 18-19 January, 2014.

5.5. Research Interests : Quantum mechanical methods based molecular modelling

5.6. Papers published in reviewed journals :

| S.No | Title of the Paper | Journal Name Vol.No. PP | ISBN/ISSN No. | Impact Factor/ Citation Index | National/ International |
|---|---|---|---|---|---|
| 1 | Theoretical insights into interaction energy, IR intensity and Raman activity enhancements of $H_2O$ adsorbed on Mg containing $Zn_3O_3$ nanoclusters: A computational study | J. Comput. Theor. Chem. | 2210-271X | 1.926 | International |
| 2 | Influence of the Effect of the Number, Nature and Position of Methyl Posttranscriptional Modifications on Nucleobase Stacking in RNA | ChemPhysChem 2021 | 1439-4235 | 3.144 | International |
| 3 | An APT charge based descriptor for atomic level description of chemical Raman enhancement by adsorption of 4-Mercaptopyridine on semiconducting nanaoclusters: A theoretical study | Vib. Spectrosc., 2020 107:103019 | 0924-2031 | 2.507 | International |

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| 4 | A DFT study on reaction force approach of ammonia catalysed amide bond formation reaction between ammonia and formic acid", | J. Mol. Graph. Model. 2020 94:107478 | 1093-3263 | 2.518 | International |
| 5 | A reaction force perspective of a model amide bond formation reaction | Comput. Theor. Chem., 2019, 1151:91-98. | 2210-271X | 1.926 | International |
| 6 | Surface enhanced Raman scattering of neutral and zwitterionic $\alpha$- and $\beta$-Proline monomers adsorbed on $Au_3$ cluster: A DFT study | Vib. Spectrosc., 2018, 98:15-21 | 0924-2031 | 2.507 | International |
| 7 | A DFT study on the role of long range correlation interaction and solvent effects in homochiral and heterochiral cyclic trimerization of imidazole based heterocyclic amino acids | J. Mol. Model., 2016, 22: 141. | 0948-5023 | 1.810 | International |
| 8 | Density functional theory based study on *cis-trans* isomerism of amide bond in homodimers of $\beta^{2,3}$- and $\beta^3$-substituted homoproline | J. Phys. Chem. A, 2014 118, 2120 – 2137 | 1089-5639 | 2.781 | International |
| 9 | Peptidomimetics with tunable tertiary amide bond containing substituted β-proline and β-homoproline", | Tetrahedron 2014 70 1169-1175. | 0040-4020 | 2.457 | International |
| 10 | Theoretical and experimental studies on solubility and reactivity behavior of lysergol, elymoclavine, and dihydrolysergol | Int. J. Quantum Chem. 2013 113 1427-1435 | 1097-461X | 2.444 | International |
| 11 | Preferential heterochiral cyclic trimerization of 5(aminoethyl)–2-furancarboxylic acid (AEFC) driven by noncovalent interactions | J. Mol. Graph. Model. 2012 38 13 – 25 | 1093-3263 | 2.518 | International |

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| 12 | Inter- versus intra-molecular cyclization of tripeptides containing tetrahydrofuran amino acids: a density functional theory study on kinetic control | J. Mol. Model. 2012 18 3181-3197. | 0948-5023 | 1.810 | International |
| 13 | A theoretical study on interaction of proline with gold cluster" | Bulletin of Materials Science 2012 35 291-295. | 0973-7669 | 1.783 | National |
| 14 | Stereochemical control in the structures of linear δ,α-hybrid tripeptides containing tetrahydrofuran amino acids | J . Phys. Org. Chem. 2011 24, 720-731. | 1099-1395 | 2.391 | International |
| 15 | Preferential mode of cyclization of tetrahydrofuran amino acids containing peptides: some theoretical insights | J. Phys. Org. Chem. 2010 23, 238-245. | 1099-1395 | 2.391 | International |