

Curriculum Vitae



Dr. ANJALI

Ph.D. Chemistry

National Institute of Technology Kurukshetra

Haryana-136119, India

Personal Information

- **E-mail:** anjalimaan20@gmail.com
- **Mobile:** +91-9671572590
- **DOB:** 20/08/1996
- **Language:** Hindi, English
- **Nationality:** Indian
- **Gender:** Female
- **Marital Status:** Married

Research Area of Interest

I am an experienced researcher in Computational Organic Chemistry by using DFT calculation is my core research area. In this regard, during the Ph.D. work, I have worked on Design and study of Nitrogen-rich High Energy Organic Explosive Materials and their Structure-activity Relationship. Further I am ready to take new challenges and always keen to learn new science.

Educational Qualification

- ❖ **Doctor of Philosophy (Ph.D.):** Computational Organic Chemistry (2020-2024), Department of Chemistry, National Institute of Technology Kurukshetra, Haryana.
 - **Guide:** Dr. Vikas Dasharath Ghule
 - **Thesis topic:** *Computational Exploration of High-Performance and Low Sensitivity Energetic Compounds based on Versatile Functionalization of Nitrogen-rich Heterocycles.*
- ❖ **Master of Science (M.Sc.):** Organic chemistry (2018), Kurukshetra University, Kurukshetra, Haryana, (First division: 79%)
- ❖ **Bachelor of Science (B.Sc.):** Physics, Chemistry, Mathematics (2016), Kurukshetra University, Kurukshetra, Haryana, (First division: 76%)
- ❖ **Senior Secondary (12th):** Science (2013), Arya Adarsh Sr. Sec. School, Ballah, Karnal, Haryana (HBSE, First division: 78%)
- ❖ **Higher Secondary (10th):** Science (2011), Pashupati Nath Public School, Ballah, Karnal, Haryana (HBSE, First division: 79.8%)

Computational Skill-----

- **Computer Knowledge:** Microsoft Office, Power-Point presentation, and Grammarly.
- **Software Knowledge:** Chems sketch, ChemDraw, Origin, Chemcraft, Gaussian, Multiwfn, Visual Molecular Dynamics, Autodock Tools, Autodock4, AutoVina, Discovery Studio, PyMol, Avogadro, Mendeley.
- Deep knowledge about Quantum chemical calculations using Gaussian program via density functional theory (DFT).

Experimental Skills-----

- Organic synthesis.
- UV/IR Spectrophotometer, NMR, Rotary evaporator,
- Distillation, Recrystallization, Column/Thin layer chromatography.

Academic Achievements-----

- Qualified National Eligibility Test (**NET**) conducted by CSIR India: June 2019
- Awarded Junior Research Fellowship (**JRF**): 2020-2022
- Awarded Senior Research Fellowship (**SRF**): 2022-2024

Detailed list of Published articles-----

1. **Anjali Maan**, Vikas D. Ghule, S. Dharavath, Computational manifestation of nitro substituted tris(triazole): understanding the impact of isomerism on performance-stability parameters, *Journal of Physical Chemistry A*, **2023**, 127, 31, 6467–6475, DOI: 10.1021/acs.jpca.3c03483.
2. **Anjali Maan**, R. Devi, Vikas D. Ghule, S. Dharavath, Design and computational studies on energetic compounds composing bridged bis triazolo-triazine framework, *Chemical Physics*, **2023**, 571, 111939, DOI: 10.1016/j.chemphys.2023.111939.
3. **Anjali Maan**, Vikas D. Ghule, S. Dharavath, Computational evaluation of polycyclic bisoxadiazolo-pyrazine backbone in designing potential energetic materials, *Polycyclic Aromatic Compounds*, **2022**, 43,8, 6717-6729, DOI: 10.1080/10406638.2022.2124282.
4. **Anjali Maan**, Vikas D. Ghule, S. Dharavath, Computational assessment of nitrogen-enriched, stable and insensitive tris(1,2,4,5-tetrazin-3-yl)amine building block for energetic applications, *Energetic Materials Frontiers*, **2021**, 3, 47-52, DOI: 10.1016/j.enmf.2021.11.002.
5. **Anjali Maan**, Vikas D. Ghule, S. Dharavath, Tetranitro-diazinodiazines as high energy materials: computational investigation of structural aspects of fused heterocyclic backbone and isomerism, *Structural Chemistry*, **2021**, 32, 2175–2181, DOI: 10.1007/s11224-021-01791-1.

6. **Anjali Maan**, R. S. Mathpati, Vikas D. Ghule, S. Dharavath, Effect of multiple oxadiazole rings with nitro and nitramino functionalities on energetic properties: computational analysis of the structure–property relationship, *New Journal of Chemistry*, **2021**, 45, 7368-7376, DOI: 10.1039/d1nj00738f.
7. **Anjali Maan**, R. S. Mathpati, Vikas D. Ghule, Energetic Triazolo-Triazolo-Furazano-Pyrazines: A Promising Fused Tetracycle Building Block with Diversified Functionalities and Properties, *ChemistrySelect*, **2020**, 5, 8557-8561, DOI:10.1002/slct.202002440.
8. **Anjali Maan**, R. S. Mathpati, Vikas D. Ghule, Substituted triazolo-triazine derivatives as energetic materials: a computational investigation and assessment, *Journal of Molecular Modeling*, **2020**, 26, 184, DOI:10.1007/s00894-020-04455-9.
9. R. Devi, **Anjali Maan**, Vikas D. Ghule, S. Dharavath, Functionalization of fused imidazole-oxadiazole, triazole-oxadiazole and tetrazole-oxadiazole skeletons: Search for stable and potential energetic materials, *Computational and Theoretical Chemistry*, **2023**, 1229, 114352, DOI: 10.1016/j.comptc.2023.114352.
10. Kalpana Sharma, **Anjali Maan**, Vikas D. Ghule, S. Dharavath, Azo-bridged Triazole Macrocycles: Computational Design, Energy Content, Performance and Stability Assessment, *Journal of Physical Chemistry A*, **2023**, DOI: org/10.1021/acs.jpca.3c05732.

Conferences and Workshop Attended-----

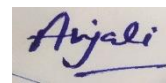
1. Presented poster in International Conference on “**Molecules and Materials Technology**” (MMT-2023) organized by NIT Kurukshetra, Kurukshetra, Haryana, India.
2. Presented poster in National Conference on “**Contemporary Facets in Organic Synthesis**” (CFOS-2022) organized by IIT Roorkee, Roorkee, Uttarakhand, India.
3. Attended international conference on “**Recent Advancements in Chemical Science**” (2021) organized by J.C BOSE University of Science and Technology, YMCA, Faridabad, Haryana, India.
4. Presented poster in International Conference on “**Innovations in Science, Engineering & Technology** (ICISSET-2019) organized by Arya Post Graduate College, Panipat, Haryana, India.
5. Workshop Attended On “**Computational Structure-based Screening and Explicit Molecular Dynamics**” (2021) organized by IIT-Kanpur and Schrodinger inc.

Reference Details-----

1. **Dr. Vikas Dasharath Ghule** (Assistant Professor)
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2. **Dr. Srinivas Dharavath** (Assistant Professor)

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A small, square image showing a handwritten signature in blue ink. The signature appears to be 'Anjali' with a horizontal line underneath.

Date: 13/07/2024

(Ms. Anjali)