Dedicated to my family

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Publications based on the research work

1. A theoretical charge density study on nitrogen-rich 4,4’,5,5´-Tetranitro-2,2´-bi-1H-imidazole (TNBI) energetic molecule.

2. Charge density distribution, Electrostatic properties and the Sensitivity of High energetic 2,4,6-Trinitro-1,3,5-triazine molecule: A theoretical study.

3. Crystal density prediction, charge density distribution and the explosive properties of high energetic 2-Methyl-5-nitroamino-tetrazole molecule: A theoretical study.

4. *Ab initio* crystal structure and understanding the bond strength of high energetic 2,4-Dinitro benzoic acids molecule via Quantum chemical calculations and charge density analysis.

5. Crystal density, charge density distribution, impact sensitivity and explosive properties of high energy nitrogen rich linear N_{10} molecules: A density functional and AIM study

6. Exploring crystal density, charge density and explosives properties of 2,6-Diamino-3,5-dinitropyrazine-1-oxide (LLM-105) energetic molecule - A computational study.
7. Ab initio crystal structure and density prediction, charge density and impact sensitivity analysis of high energetic 4-Amino-3,5-dinitro-1H-pyrazole molecule.

P. Srinivasan, S. N. Asthana and Rajesh B. Pawar and P. Kumaradhas, 
(Manuscript under preparation)

8. Bond topological, electrostatic and thermo chemical properties of 2,4,6-Trinitro-2,4,6-triazaheptane (ORDX)–A Computational study.

P. Srinivasan, S. N. Asthana and Rajesh B. Pawar and P. Kumaradhas, 
(Manuscript under preparation)

**Publications related to the research work**

1. Bond charge depletion, bond strength and the impact sensitivity of high energetic 1,3,5-Triamino 2,4,6-trinitrobenzene (TATB) molecule: A theoretical charge density analysis.


2. Exploring the bond topological and electrostatic properties of Benzimidazole molecule via Experimental and theoretical charge density study.


3. Effect of gold atom contact in conjugated system of one-dimensional octane dithiolate based molecular wire: A theoretical charge density study.


4. Ab initio crystal structure prediction and the charge density distribution of high energetic Dimethyl nitraminotetrazole: A first step for design of high energy density material.

Thesis work contributed in conferences/seminars/workshop


