Explosive materials power critical sectors from national defense to space propulsion, yet their development is hampered by a persistent trade-off: increases in energetic performance frequently elevate sensitivity, complicate manufacture, and undermine sustainability. This dissertation confronts that trade-off by establishing a unified, data-driven discovery platform that combines prospective machine-learning guidance, modular synthetic design, and rigorous experimental validation to deliver high-performance energetic materials that retain thermal stability, processability, and safer handling.

This work presents the design, synthesis, and characterization of a family of molecules engineered as next-generation melt-castable energetics. A modular, nitration-controlled synthetic route was developed to maximize yield and minimize hazardous steps, using prospective machine-learning property predictions to guide design. Experimental evaluation confirms favorable thermal stability, processing behavior, and low mechanical sensitivity, while comparison of predicted and measured properties highlights both the reliability and current limitations of descriptor-based models. Integration of these findings into the computational workflow establishes a closed-loop discovery framework in which iterative feedback refines model accuracy and accelerates targeted molecular design.

The dissertation also introduces a fundamentally new class of covalently functionalized multi-walled carbon nanotubes bearing tetrazole-based moieties. This nanocomposite platform enables tunable energetic release and photothermal response, producing rapid, localized heating and controlled gas generation under near-infrared irradiation. The system integrates photothermal and chemical energy conversion within a programmable nanoscale architecture and, beyond energetic applications, offers a pathway toward targeted, noninvasive therapeutic approaches by enabling precise control of light-triggered heat and reactive-species generation. Though preclinical, this multifunctional conjugation strategy links energetic chemistry and biomedical innovation through a unified molecular design principle.

Additional studies expand the scope of the work to address key process and application challenges: (i) an energy-efficient laboratory synthesis of high-purity calcium cyanamide is demonstrated as an improved alternative to the traditional Frank–Caro route; and (ii) an isocyanate-bearing mechanophore is developed and validated for mapping stress distribution in propellant matrices, providing a chemical reporter that links mechanical loading to chemical activation and failure.

Together, these studies establish a scalable, data-driven pathway for creating safer, more manufacturable energetic materials and adaptable nanotechnologies, with transformative potential across defense, space propulsion, and biomedical sectors.