AVT-340 Research Workshop on Preparation and Characterization of Energetic Materials

Office of Naval Research Advanced Energetic Materials Program Overview

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3 February 2021

Code 35, Aviation, Force Protection, and Integrated Defense

Aerospace Sciences Division (351). Focuses on strike technology. Basic and applied research projects include energetics, autonomy, hypersonics, rotorcraft technology, advanced propulsion naval air and surface weaponry, and naval aircraft that could provide transformational capabilities for the Navy After Next.

Air Warfare and Weapons Applications Division (352). Naval unique or essential projects in this division are involved with applied research and advanced technology aligned with current and future naval capability gaps and innovative naval prototypes.

Air Platforms
- Aerodynamics
- Flight Dynamics and Control
- Aviation Structures and Materials
- Aircraft Propulsion
- Autonomy

Kinetic Weapons
- Advanced Energetic Materials
- Hypersonics
- Air Weapons
- Electromagnetic Rail Gun INP (EMRG)

Directed and Counter Directed Energy (DEW/CDEW) Weapons
- Lasers and High Power Microwaves
- Solid State Laser Technical Maturation INP (SSL-TM)
- Rugged High Energy Laser INP (RHEL)
- High power Joint Electromagnetic Non-Kinetic Strike INP (HIJENKS)

Advanced Energetic Materials

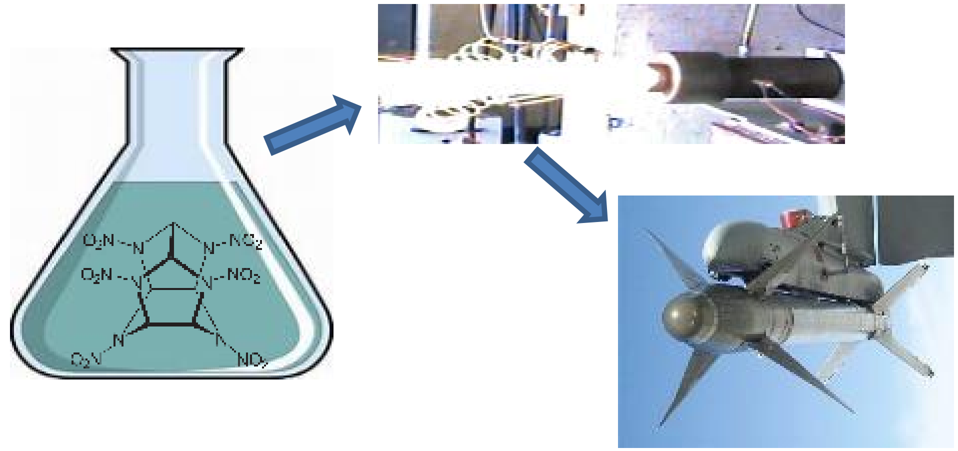
Program Objective: Naval power projection with safe, cost-effective ordnance with precision & adaptable effects (all domains)

Program Approach: Enhanced performance and safety for weapon systems:

- New energetic materials and energetic material concepts to enhance warhead and propellant performance
- Novel dynamic diagnostics development and implementation – understanding complex energy release
- Atomistic through continuum level predictive solutions – properties prediction, performance, IM requirements composite design, lethality
- Reduced energetic material sensitivity to initiation by external unplanned stimuli without reducing performance

Program Payoff:

- Increased lethality, range, and speed of munitions
- Improved safety and reduced vulnerability
- Weapon Integration



Advanced Energetic Materials Program:

- Resides within Code 351 – Aerospace Sciences Division, DE/CDE, RG, Autonomy, Aerodynamics, Advanced Propulsion, Hypersonics….Energetic Materials
- Leverages with other ONR codes (352, 33, ONRG), services (Army, AF), funding agencies (DTRA, DARPA, DHS, MDA, etc.), and OSD joint programs (DoE/JMP, JEMTP)
- Balances S&T with warfighter needs in terms of energetic materials

Funding Profile:

- 6.1 Core – Academia (training future S&T workforce)
- 6.2 Core – Navy/DoD Labs, Industry
- Non-Core: YIP, DURIP, MURI, SBIR/STTR, congressional adds
- 6.3 – Future Naval Capabilities (FNC), Innovative Naval Prototypes (INP)

Performers:

- **Academia:** UC Santa Barbara, Purdue, LMU Munich, U. Michigan, Temple, Washington State, Texas Tech, Stanford, U. Virginia, MIT, Hawaii, NJIT, U. Florida, U. Maryland, Cal. Tech., Georgia Tech, Brown, Scripps, Cornell, Johns Hopkins, Utah, UC Berkeley, Harvard, U. South. Cal., Northeastern, CSU Long Beach
- **US Navy/DoD/Industry:** NSWC IHEODTD ,NAWC WD, NSWC DD, NSWC Crane, NPS, NRL, USNA, ARL, SRI International, Northrup Grumman, various SBIR/STTR partners

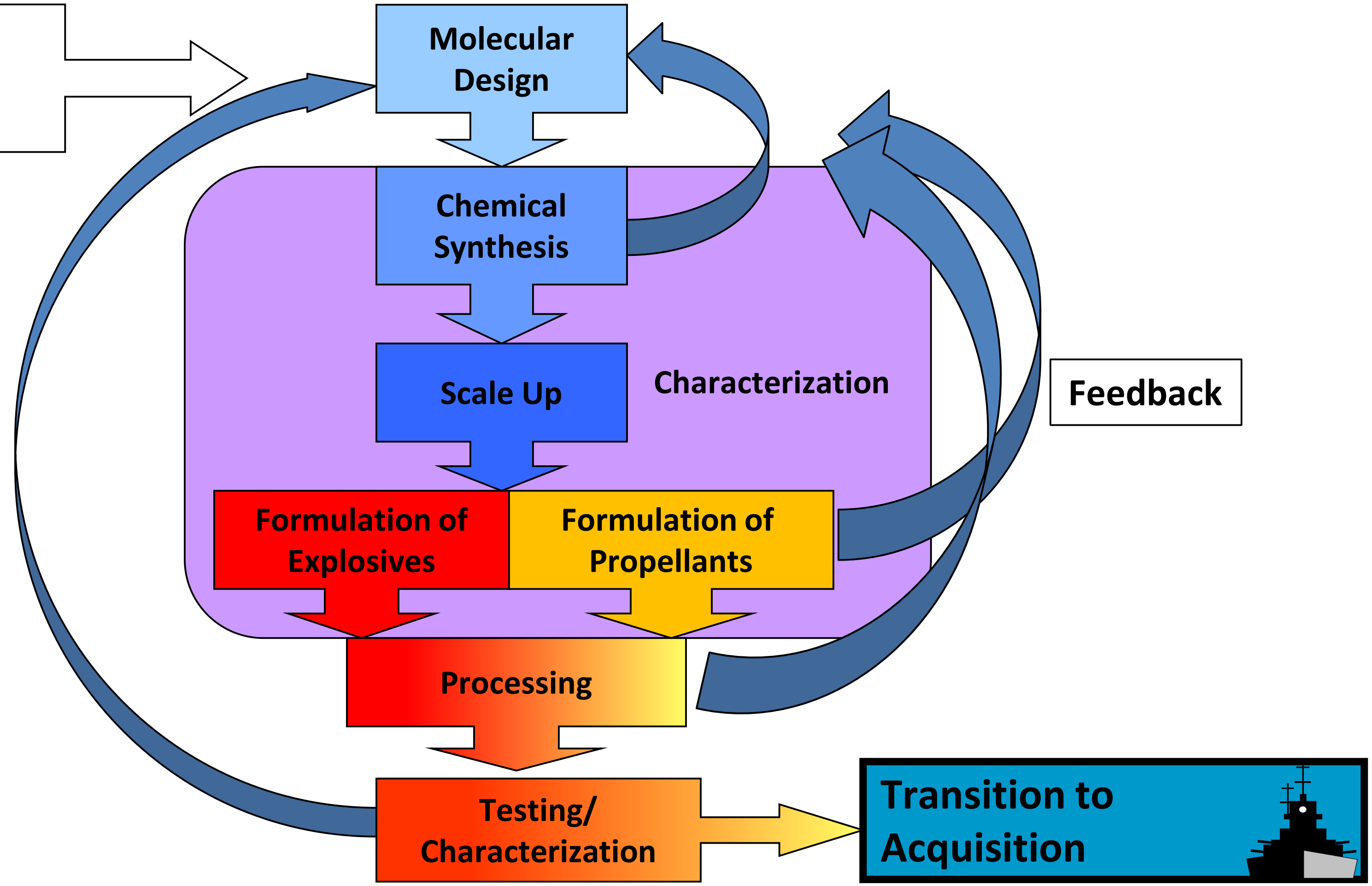
Broad Thrust Areas

- **Tactical Propulsion:**
  - Higher performance – range and speed
  - need to be able to use the energy more efficiently
  - need to control energy release better (on/off propulsion?)
  - walk the line between kinetic stability and increased energy release rates

- **Explosives/Effects:**
  - need to couple energy output to targets more effectively
  - Higher energy? Or selectable energy?
  - Smaller package, same or greater lethality
  - Maintain IM properties

- o All of this requires fundamental understanding and combined efforts: new ingredients, new formulations, advanced diagnostics, modeling/simulation
- o Technology push vs. technology pull (demand signals?) – OPNAV/PEO
- o Examples of Transition Partners include DTRA, OSD (JEMTP, JMP), other Navy (ONR/NSWC), PEO IWS 3, IWS 11, PEO U&W, PMA 201, PMA 242, Navy SSP, USMC PM AMMO

Explosives/Propellants Development Cycle (6.1/6.2/6.3)



Good: Development cycle provides feedback for S&T efforts

Bad: Process historically takes decades – need comprehensive understanding & predictive capabilities

S&T Thrust Areas

Molecular Design/Synthesis/Ingredients:

- High energy density explosives/oxidizers, (solid) fuels, cage structures (ex. CL-20)
- Enabling materials: polymers/binders, burn rate modifiers, plasticizers, catalysts, composite materials, new concepts
- Exotic ingredients/materials amenable to special applications, ex. Reactive Materials (RM), Additive Manufacturing (AM)
- Formulation studies – all domains

Detonation, Combustion & Propulsion Diagnostics:

- Shock physics, detonation science, novel combustion phenomena
- Ignition, kinetics/mechanisms, stability/reactivity, formulations/IM
- Characterize/push ingredient transitions and feed/validate modeling

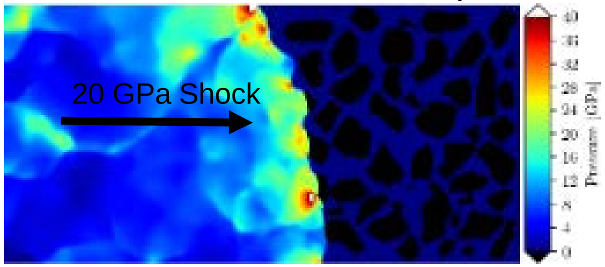
Computational QM → Continuum Modeling

- Atomistic to Mesoscale, material properties, behavioral predictions
- Predict performance/stability, model lethality, maintain IM
- Drive synthesis, draw from/drive diagnostics, predict effects

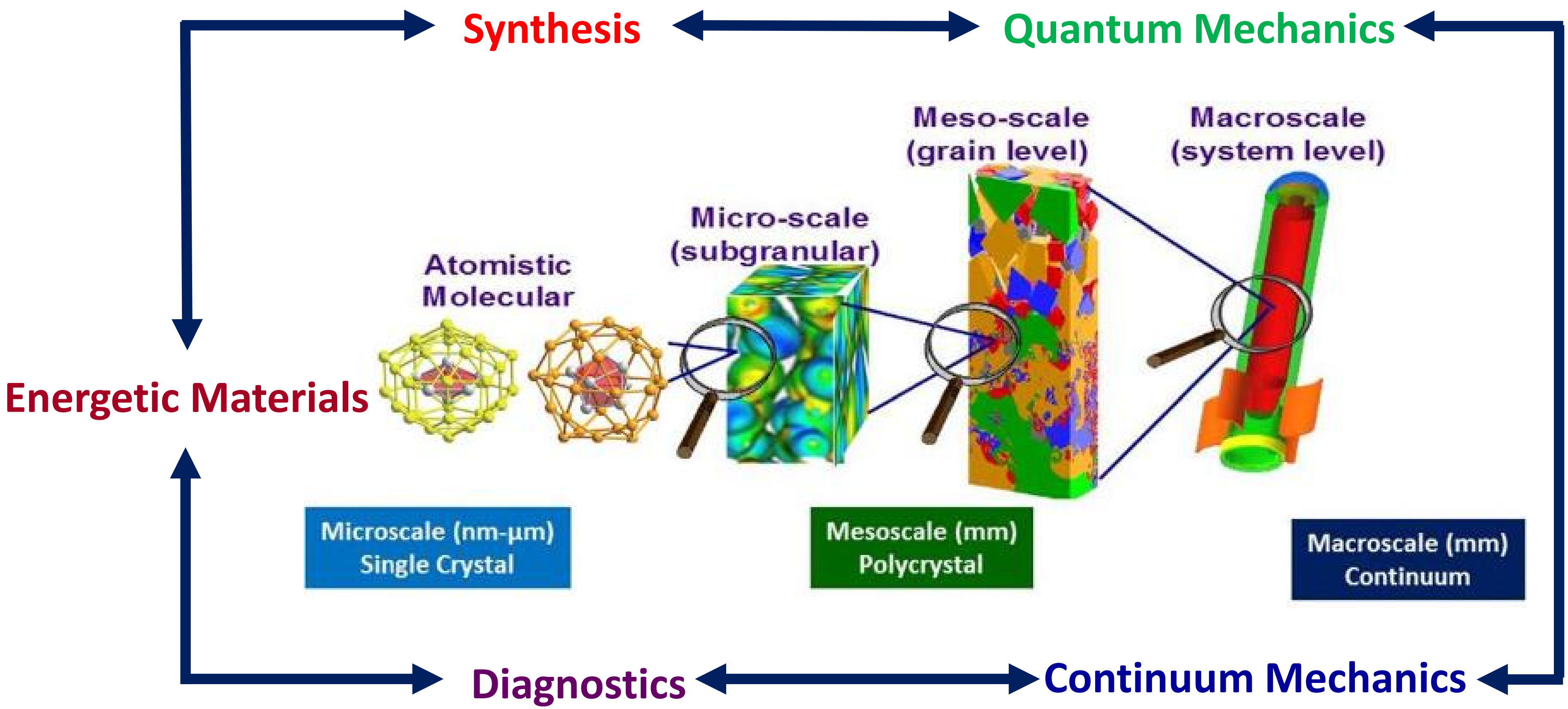
6.1		6.2
Methodology	→	Targets/scale up
Polymer Chem.	→	Formulations
Interfac. Interact.		

Diag. Develop.	→	Shock/Det. Sci.
Combustion	→	Propulsion

Atomistic Sim.	→	Mol. Properties
Multiscale Mod.	→	Lethality Codes



Advanced Energetic Materials Investment Strategy



Key Questions:

- What drives the reaction chemistry?
- What stabilizes ignition and growth?
- What desensitizes global reaction?

Work Across Research Domains is Essential for Progress

6.1 (Basic Research)Topic Areas

Materials/Synthesis:

- Synthetic methodology, structure property relationships, new ingredient types
- Controlling binder polymerization/cure chemistry, new fuel/oxidizer concepts
- Enabling emerging technologies: Additive Manufacturing of energetics, microfluidics synthesis, etc.

Diagnostics/Experimentation:

- Diagnostics method development → what tools does the US DoD need?
- Experiments at extreme conditions → high T, high P diagnostics
- Fast time scales, fundamental mechanistic/kinetic understanding
    - Ingredients and composites

Modeling/Theory:

- Predict: Material Properties, Performance, Insensitive Munitions (IM) response
- Meso-scale/multiscale/continuum modeling → feed 6.2 efforts

Feed 6.2 research in US DoD Labs: Scale up, Explosive/Propellant Formulations

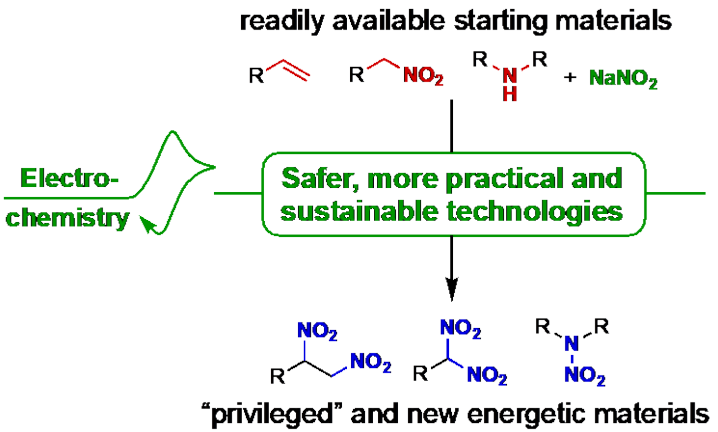
6.1 Program Diversity

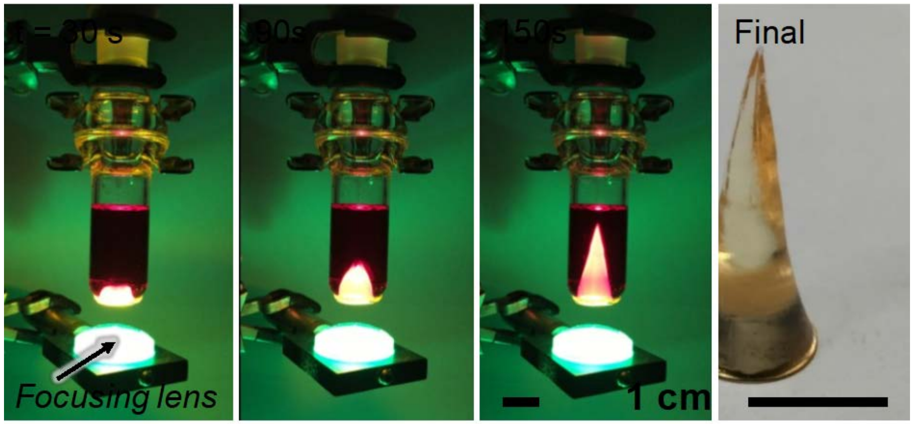
- Highly-Strained Heterogeneous Cyclics (Scripps, Baran)
- Enhancing Mechanical and Combustion Properties of Boron/Polymer Composites via Engineered Interfacial Chemistry (Stanford, Zheng & Xia)
- Increasing Energy Density by Creating Redox Frustration in Hybrid Organic/Inorganic Energetic Materials (Temple, Zdilla)
- Advanced Energetic Materials New route of Tetrazine dioxide Heterocycle Synthesis Opening up new Very High Performing Energetics (Purdue, Piercey)
- Pre-Stressing Metal Fuel Particles for Enhanced Reactivity (Texas Tech, Pantoya & Iowa State, Levitas)
- Ammonium Dinitramide Cocrystals for Improved Performance and Environmental Stability (University of Michigan, Matzger)
- Safe Synthesis of Explosives on demand via Microreactor Techniques (University of Munich, Klapötke)
- Crystalline/Molecular Mechanisms Governing Structural and Chemical Changes in Shocked HE Single Crystals – Real-Time, Multiscale Measurements (WSU, Gupta)
- Real-Time Measurement of Physical and Chemical Evolution of Energetic Materials Under Shock Loading (MIT, Nelson)
- Molecular Engineering using Solution Shearing for Enhanced Stability and Performance of Energetic Materials (UVA, Giri)
- Multi-Scale Methods to Simulate Detonation and Deflagration in High Density Propellants (Georgia Tech, Menon)
- Reactive Dynamics Modeling and Simulations to Predict Structures, Physicochemical Properties, Initiation Kinetics, and Performance of Novel Energetic Materials and Composites (CIT, Goddard)
- YIP - Electrochemical Methods for the Installation
- of N-containing Explosophores (Cornell, Lin)
- YIP - Selective Alkene Functionalization as a Platform for Energetic Materials Development (Scripps, Engle)
- MURIs – Metalloid Clusters; Predictive Chemistry & Physics @ Extreme Conditions; Synthesis Planning; Organic Molecular Decomposition (new start)

6.1 Highlights – Synthesis/Materials

Novel Synthetic Electrochemical Nitrations Simplifying Synthetic Routes for Existing Energetics and Opening New Arenas for Discovery

Cornell University, Lin

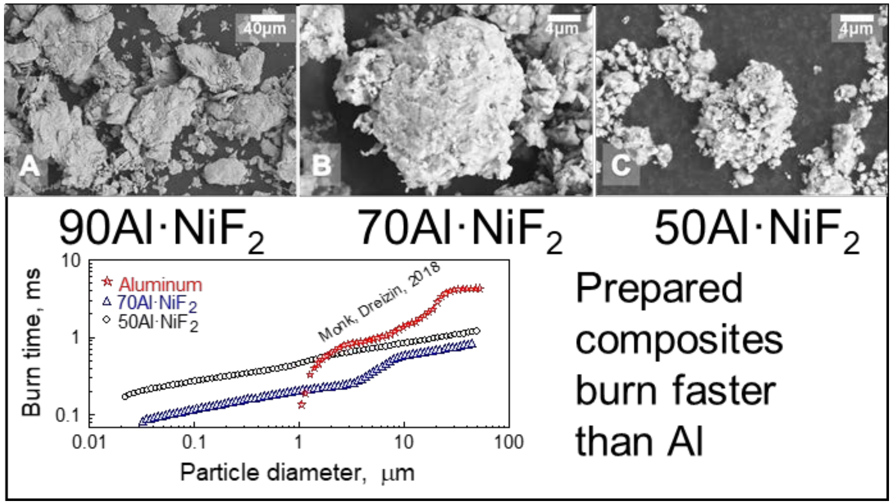




Design of New Polymer Binders for Additive Manufacturing

UC Santa Barbara, Read de Alaniz

6.1 Highlights – Diagnostics

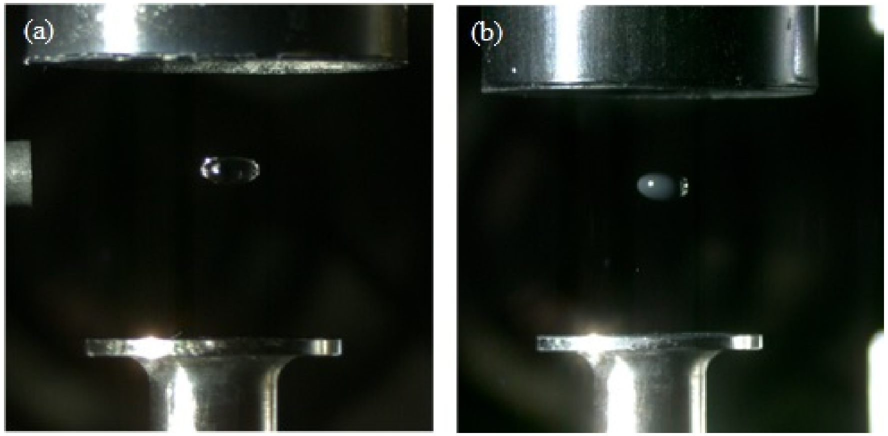


Reactive Fluorinated Composites for Advanced Energetic Systems

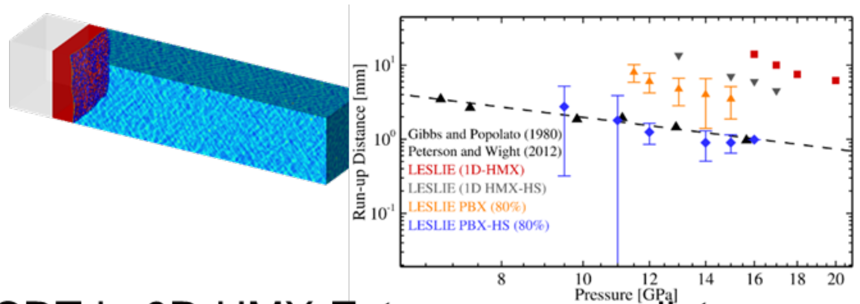
NJIT, Dreizin

Spectroscopic Study of the Reaction Mechanisms of the Oxidation of (JP-10) in Levitated Droplets

University of Hawaii, Kaiser



6.1 Highlights – Modeling/Theory



SDT in 3D HMX-Estane; run-up distance
Predicted using hotspot model and UQ

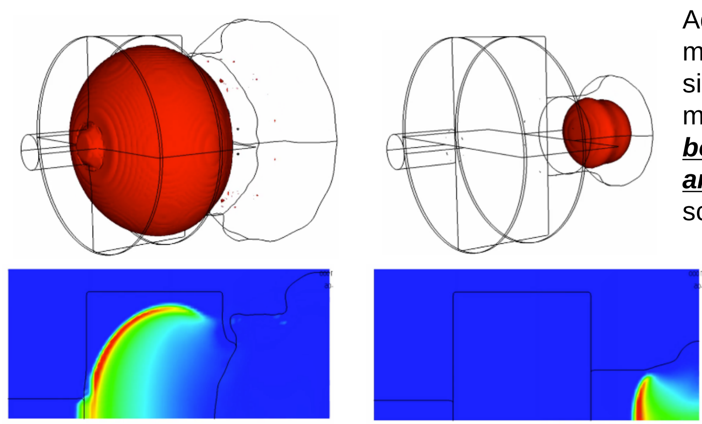
Multi-Scale Methods to Simulate Detonation and Deflagration in High Density Propellants

Georgia Tech, Menon

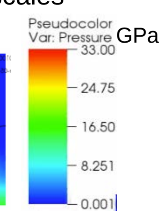
Continuum Modeling of Energetic Materials to Interpret Atomistic and Molecular Simulations for Advanced Design

University of Florida, Stewart

Stewart-Group: Advanced Simulation of Explosive Systems



Advanced multi-material simulation and modeling at ***both*** system ***and*** nano-scales



6.2 (Applied Research) Topic Areas

Ingredients

— New High energy density explosives/oxidizers, Fuels, New polymer/cure technologies
— Ingredient scale-up, testing viability for practical use
— Optimization/cost reduction

Process Research and Formulations

— Explosives/propellants formulation with emerging ingredients
— Novel manufacturing (Flow, AM and Resonant Acoustic and other mixing technologies

Novel (Enhanced Lethality) Warhead Concepts

— Reactive Materials (RM), Enhanced Blast Materials

Tactical Propulsion (Range/Speed/Maneuverability)

— High performance solid rocket motors, air breathing propulsion

Applied Diagnostics/Combustion/Shock/Detonation Science (warheads/propellants)

— Lab scale, Bomb-proof, gas/powder gun, large-scale field testing and experimentation

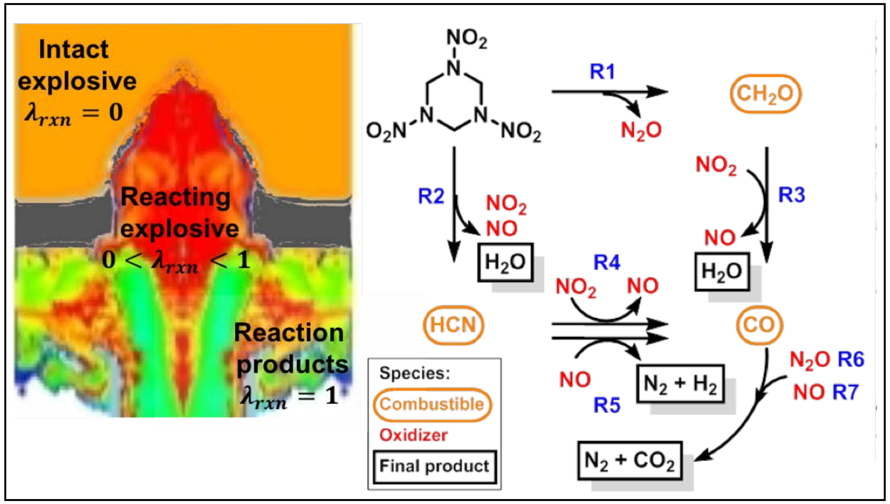
Meso-scale/Multi-scale modeling

— To examine everything from ingredient/formulation properties predictions, shock wave interactions, Lethality predictions, propellant combustion, IM response, munitions lifecycle

Performed by DoD/Navy Laboratories/Industry/SBIR/STTR

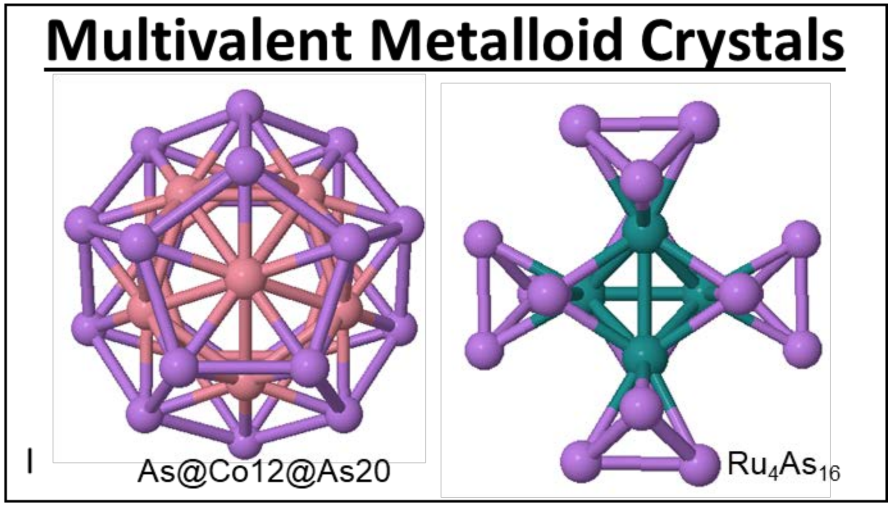
GOAL: TRANSITION → Program of Record → FLEET (FNC, INP, etc.)

6.2 Highlights



Reaction Kinetics and Energy Release in Nitramine-based Explosives

Naval Research Lab, Schweigert



Self-Assembly of Particularly Stable Metalloid Cluster Materials

Naval Research Laboratory, Palenik

Parting Considerations

- Technical considerations:
  - Where are the MOST fruitful future investments?
  - What is achievable? (near term vs. far term S&T)
  - Near term reality vs. “moon-shots” (technical rigor)
  - The periodic table isn’t changing anytime soon
  - Controlling energy release (kinetics) vs total available energy

- Less Technical considerations:
  - S&T to Acquisition pathways, cognizance of warfighter needs
  - Interaction between S&T programs 6.3 & up → 6.2 → 6.1 direction
  - Balancing innovation and training/work force development
  - How to shorten the acquisition cycle?

Summary

The ONR AEM program is focused on increasing the performance and safety profile for a large variety of weapon and propulsion systems. Our goal is a stronger more lethal Navy; our approach is multifaceted.

Overall 6.1/6.2 Thrust Areas in support of Tactical Propulsion/Warheads are very broad and contain a great diversity of projects. These include:

- Molecular Design/Synthesis/Ingredients/Formulations
- Novel dynamic diagnostics development and implementation
- Development of atomistic through continuum level predictive solutions

Most of our 6.1/6.2 projects are collaborative and there is always potential to expand collaborations through new projects or within the current portfolio.