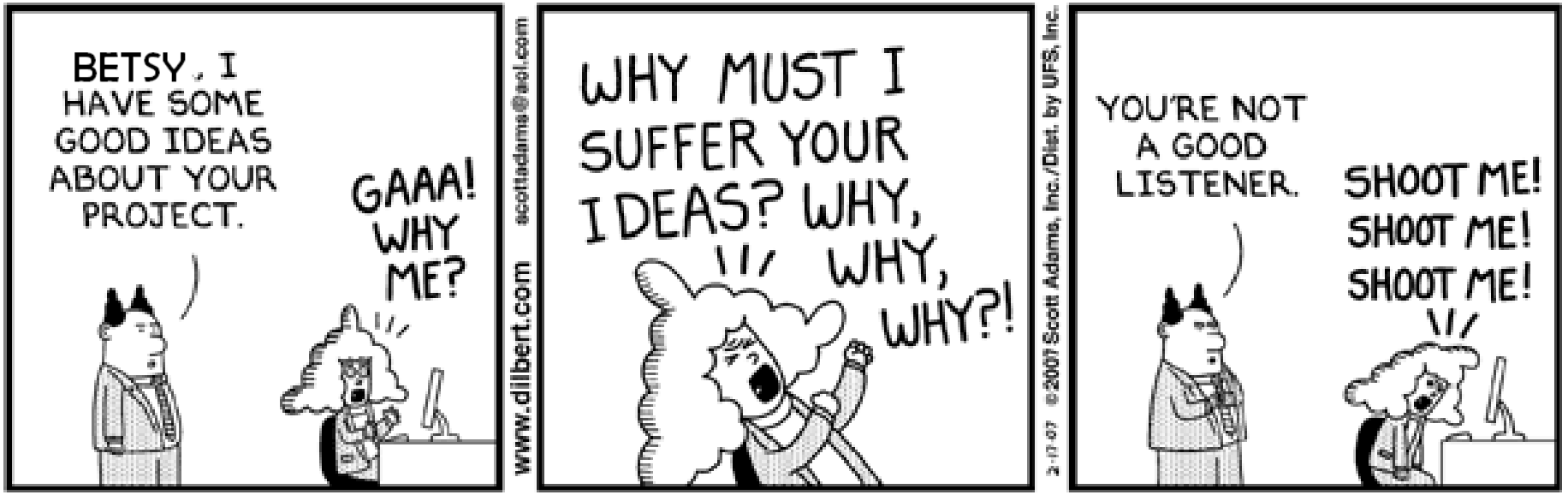
"New Ways to Store & Release Chemical Energy"

Next Generation Energetic Materials

Drs. Brad Forch & Betsy Rice
U.S. Army Research Laboratory
Weapons & Materials Research Directorate

Energetics Research Facility

Brad's Planning for Next Generation Energetic Materials



Outline . . . . . .

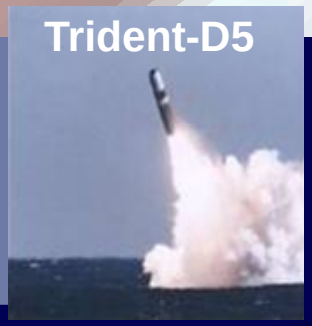
Green, Insensitive, High-Performance, Low Cost Energetic Materials??

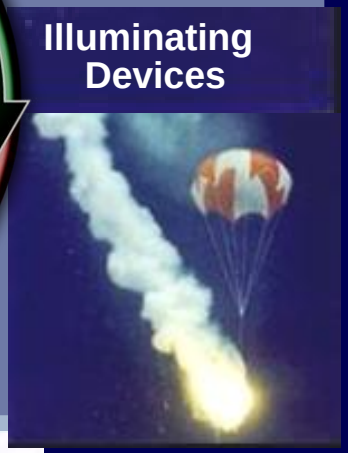
Conventional Munitions . . .

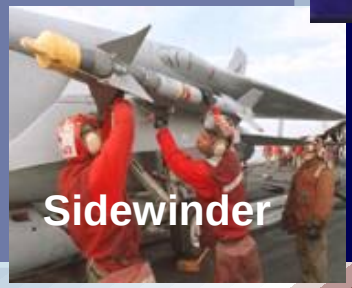
. . . and Future Munitions

- *Why Energetics?*
- *Drivers for Energetics*
- *Design Tools for Energetics & the Wise Wizard*
- *Energetic Materials Science*
- *Multiscale M&S*
- *Discussion*

There is no Military Force without Energetic Materials





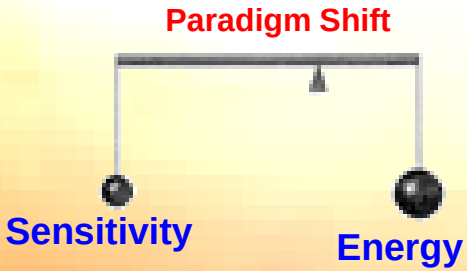



Weapons Enterprise
It's all about Energetics…and there are
Substantial Improvements that can be Achieved
Powered by
Advanced
Energetic
Materials

These are some Drivers for Energetics

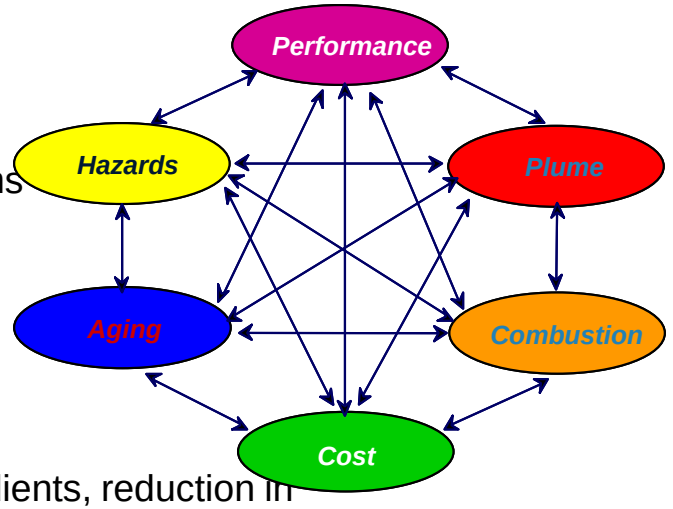
- Need for Improved Weapons Capabilities Enabling:
  - Insensitive Munitions
  - Smaller Munitions Systems
  - Enhanced Force Projection
  - Enhanced Lethality & Survivability (LW Platforms)
  - Enhanced Versatility for Multipurpose/Scalable Applications
  - Lifecycle Management – Green Technologies, Cost
- More Destructive Energy Delivered to Targets Is Critical
- Energetic Materials Provide the Chemical Energy (propellant, explosive for the Gun, Rocket, Warhead, Bomb)
- Many Possible Approaches for Energetics
  - More stored energy in explosive/propellant
  - More efficient energy conversion "MANAGED ENERGY RELEASE"
  - Higher proportion of available energy delivered to target
  - Better coupling of delivered energy to target vulnerabilities

Focus on S&T to enable Insensitive, Green, Low Cost + HIGHER PERFORMANCE



Warfighter Payoffs (Propellants)

- **Increased Lethality**
  - Enhanced system effectiveness and accuracy in smaller munition
  - Increased propellant energy and density
  - Increased ballistic impetus & variable thrust, ISP, penetration
  - Increased launch and thrust to weight
  - New kill mechanisms (multi-purpose munitions)
  - Energetic materials that are used in weapon structure (structural energetics), e.g. energetic structural cases for projectile, rocket, missile (replace intert with energetic)
- **Sustainability**
  - Common, low-cost propellant formulations
  - Greater standoff and lethal radius with less muntions
  - Allow defeat of difficult targets via new damage mechanisms
  - Soft launch of smart weapons with multiple use warheads
- **Maintainability**
  - Safety (Lower sensitivity of munitions) - CRITICAL
  - Reduced life-cycle costs (extended storage lifetime)
  - Reduced wear & erosion (barrels, nozzles)
  - Reduce support costs
  - Reduced environmental impact (e.g. less toxic novel ingredients, reduction in solvents)
- **Recognizability of kill**
  - Clearly visible damage (increased damage on target)
  - More effective kill (higher energy on target)
- **Persistent Intelligence, Surveillance, and Reconnaissance (ISR) Enabler**
  - Smaller and/or lighter payloads
  - Tailorable



Warfighter Payoffs (Explosives)

- **Increased Lethality**
  - Enhanced system performance and effectiveness in smaller envelop
  - Warhead fills that combine properties (high energy content and insensitivity; metal fragmentation capability with blast overpressure).
  - Increased energy and density
  - Increased blast, penetration, and metal accelerating capability
  - Small weapons for MOUT and complex terrains
  - Scalable effects and new kill mechanisms (multi-purpose munitions)
  - Reactive Materials - energetic penetrating and structural materials (fragments, SJC, cases, (replace inert with energetic)
- **Sustainability**
  - Common, low-cost explosive formulations (Insensitive Munitions)
  - Greater standoff and lethal radius with less explosive
  - Allow defeat of difficult/complex targets via new damage mechanisms
  - Multiple use warheads (reduce inventory requirements by 30 to 40%)
- **Maintainability**
  - Safety (Lower sensitivity of explosives for tactical, logistical storage) - CRITICAL
  - Reduced life-cycle costs (extended storage lifetime)
  - Reduce support costs
  - Reduced environmental impact, training range sustainment (e.g. less toxic novel ingredients)
- **Recognizability of kill**
  - Clearly visible damage at stand-off distances (increased damage on target)
  - More effective kill (higher energy on target)
- **Persistent Intelligence, Surveillance, and Reconnaissance (ISR) Enabler**
  - Smaller and/or lighter payloads (50% smaller and lighter (50%))
  - Tailorable

MOUT

New munitions technologies that will significantly improve a soldier's ability to fight in an urban environment

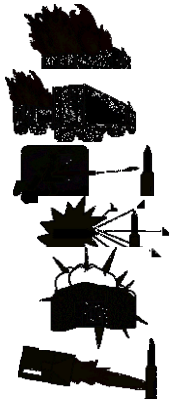
Insensitive Munitions

Objective: Develop new energetic materials, technologies and predictive tools for improving the response of gun propulsion charges, rocket motors, and warheads to threats

War Fighter Survivability

Munitions which reliably fulfill their performance, readiness and operational requirements on demand, but which minimize the probability of inadvertent initiation and severity of subsequent collateral damage to weapon platforms, logistic systems and personnel when subjected to unplanned stimuli.

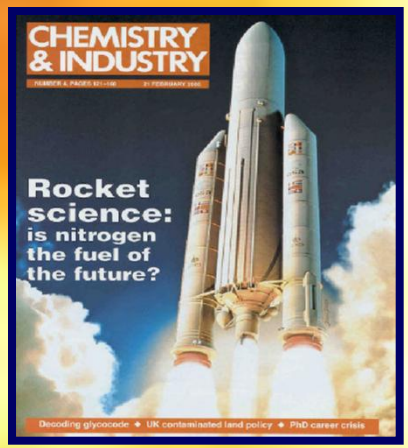
6 Tests



- ***Fast cook-off***
- ***Slow cook-off***
- ***Bullet impact***
- ***Fragment impact***
- ***Sympathetic detonation***
- ***Shaped Charge Jet Impact***

Green Insensitive, High-Performance Energetic Materials

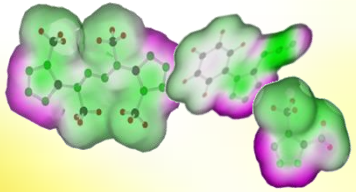
New High-Nitrogen Energetic Materials



ATTRIBUTES:

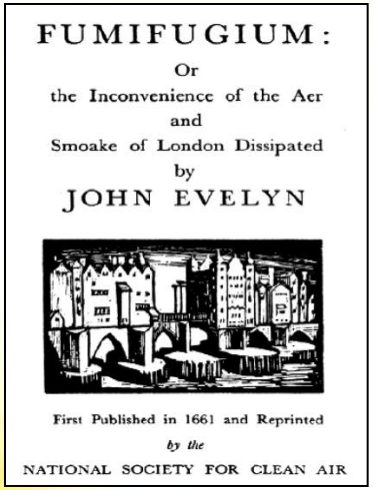
- Higher Energy
- Less Sensitive
- Smokeless, Low Signature
- Reduced Erosion (propellants)
- Only Gaseous Products (low tox)
- Rapid Environmental Degradation

Partnerships with Army, Navy, DOE, Thomas M. Klapötke, University of Munich & UMD



Theoretical Chemistry , Synthesis, and Formulation

Pollution Prevention London, 1661

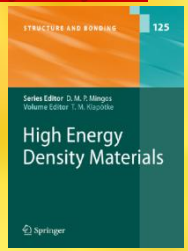

FUMIFUGIUM:
Or
the Inconvenience of the Aer
and
Smoake of London Dissipated
by
JOHN EVELYN

First Published in 1661 and Reprinted
by the
NATIONAL SOCIETY FOR CLEAN AIR

Oldest Reference I could find

CHEMICAL & Engineering News

nature



THE INDEPENDENT


Going with a greener bang

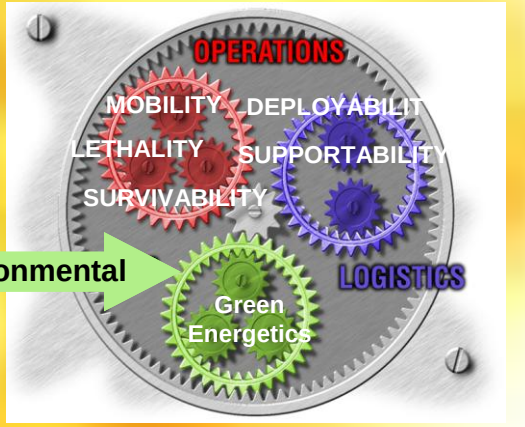
German researchers, speaking at the recent ACS meeting in New Orleans, US, have made a new class of environmentally friendly, highly energetic materials for potential use as explosives. Thomas Klapötke from Ludwig-Maximilians University, Munich, Germany, described how he and his team synthesised a new series of compounds based on

So far, Klapötke and his team have successfully synthesised hydrazinium azide hydrazinate (see right), hydrazinium azobistetrazolate hydrazinate, tetrazole azide, dinitroburet and other novel derivatives of pentazole and tetrazole. According to Klapötke, not only do the new materials contain high levels of nitrogen that are required for

EQT

Sustainment

Environmental

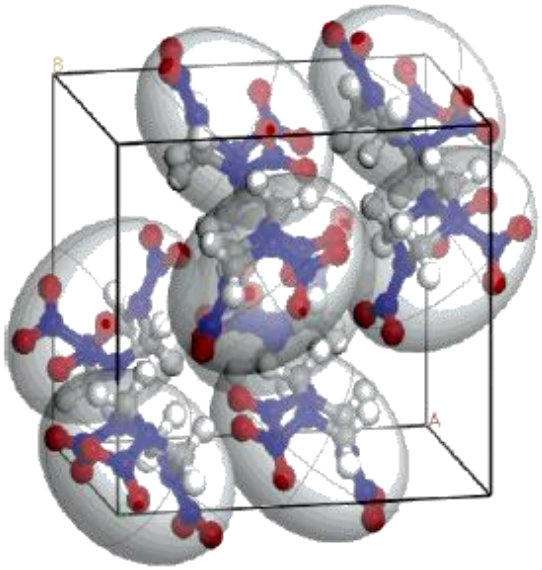


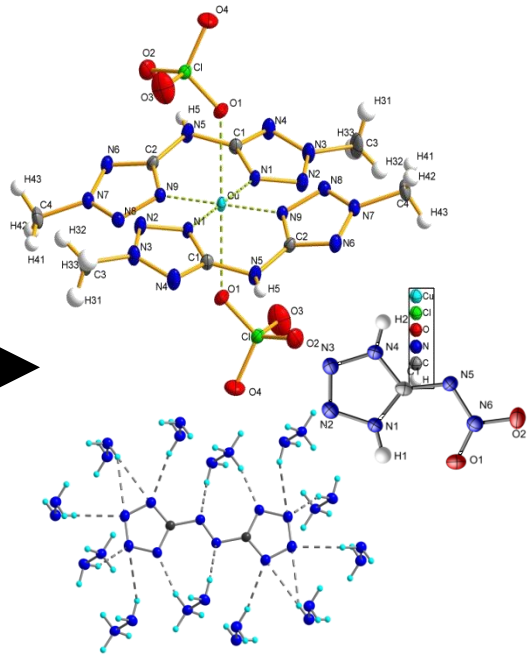
Strengthen Army operations by:

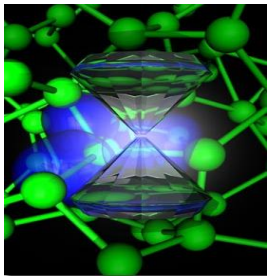
- Reducing environmental footprint
- Minimizing impacts and total ownership costs
- Sustaining test and training ranges

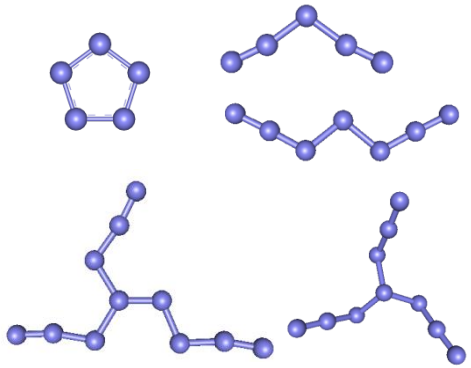
Enabling Ranges, Ammo Plants & Depots

New Energetic Materials
Many Approaches









Nitramines

High-Nitrogen
New Chemistries
New Opportunities

Metastable
Structures, Extended
Solid Energetics

Been There…

Learning This…

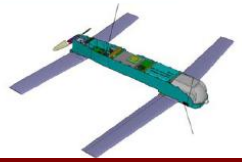
Reaching for this…

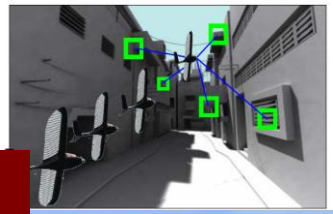
New Energetics for Swarming Multi-Agent Systems & Micro Munitions

RDECOM

Air, Ground, Undersea Autonomous

Autonomous

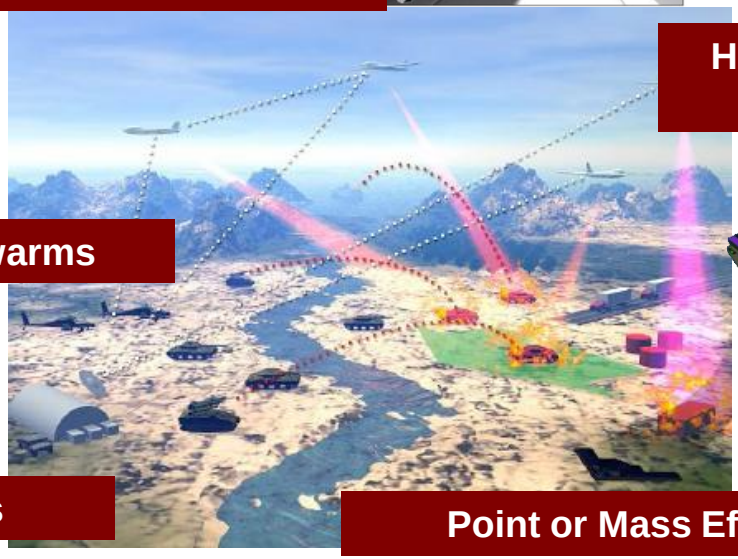




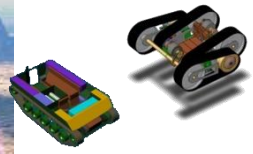
Hard to Detect & Destroy

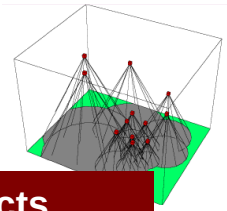
Cooperative Behavior

Swarms



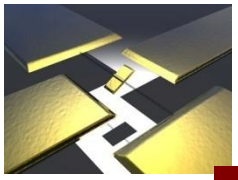
Hovering & Loiter





Zero in on Specific Targets

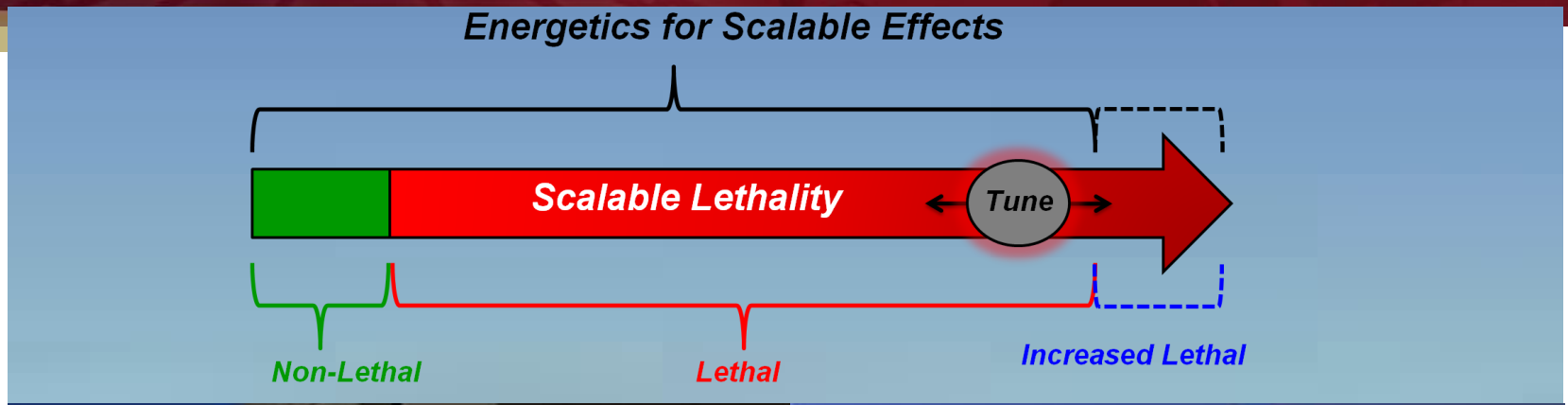
Point or Mass Effects



Nano-Motors

Very Small Weapons, alone Limited Lethality, Mass Attack of Hundreds on Single Target

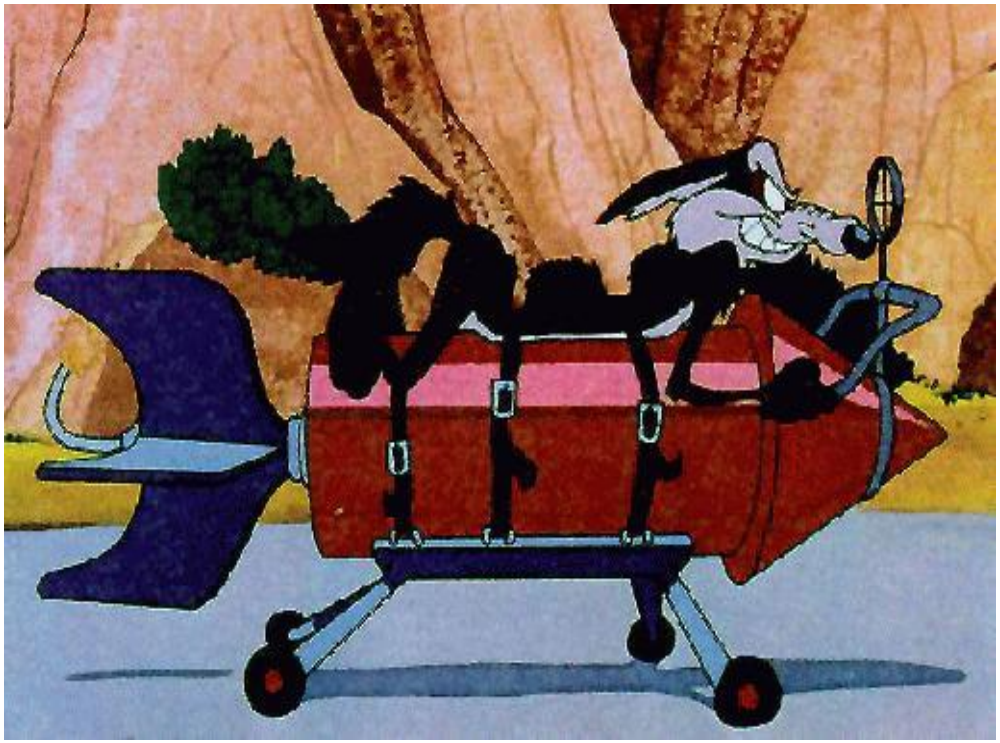
New Energetics for Scalable & Multipurpose Effects



USED.

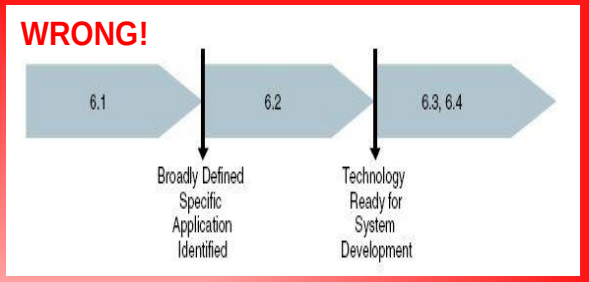
….these Technologies are Important too…

Energetics for Rockets & Missiles (Precision Guidance too)



Energetics for Gun Propulsion (Muzzle Flash too)

Research Program Elements



Basic and Applied Research
Energetic Materials

Technology Transfer

Novel Materials

- Nano-Energetics
- Nano-Materials
- Self-Assembled
- High-Nitrogen
- Ionic Liquids
- Crystal Morphology
- Crystal/Binder Interactions
- Liquids
- Gels
- Reactive Materials, Structural Energetics
- Super Atoms

Modeling & Simulation

- QM/MD Molecular Modeling
- Meso
- RX Monte Carlo
- Impact/CTH
- Detonation/CTH
- Secondary Comb/CTH
- Cyclops
- Ign & Combustion
- IB Propulsion/NGEN3
- Reactive CFD/NSRG3
- Model Coupling

Experimentation & Phenomenology

- Initiation
  - Impact/Shear
  - Thermal/FCO/SCO
  - Propagation

Energy Transfer & Partitioning

- Energy Release
- Ignition & Combustion
- Ballistic Studies
- Propellant & Explosives Studies
- Formulation
- Processing
- Advanced Diagnostics

Teaming

- RDECOM
- ONR, NRL
- AFOSR, AFRL
- DTRA
- DOE/TCG
- Universities (MURI/SIP)

Leveraging Tri-Service Basic Research in Energetic Materials

MURI

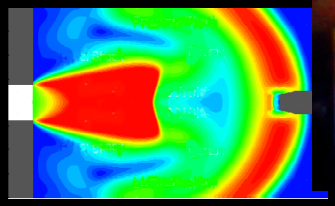
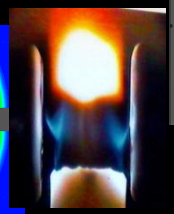
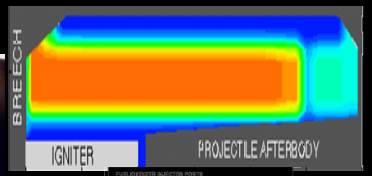
- Insensitive Munitions
- Energetics Initiation & IEDs
- Theoretical Chemistry
- Nano-Energetics & Nano-Engineered Energetics
- Wear & Erosion
- Structural Energetics & Reactive Materials for MOUT
- Hypergolic Propulsion

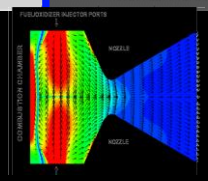
Enabling Science

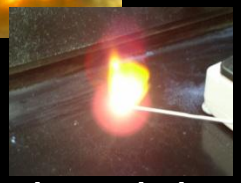
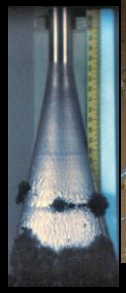
- Green insensitive energetics
- Novel propellants & explosives
- Multi-scale Modeling & Simulation
- Initiation mechanisms
- Energy transfer & propagation
- Reactive force fields
- Ignition & combustion mechanisms
- Spectroscopic techniques
- Supercritical fluid processing
- Nano-energetic materials kinetics
- Fabrication of nano-structures
- Self-assembled nano-energetics
- Chemical erosion models
- Low erosion propellants
- Low erosion weapons materials
- Reactive materials initiation models
- Fabrication of reactive materials
- Reactive materials target interactions
- Reactive materials chemistry
- Structural energetic materials
- Reactive flows, turbulent combustion

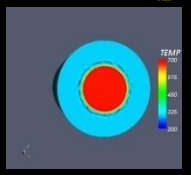
Need New Concerted Effort in Synthesis of Energetic Materials

Energetic Materials
Closely-Linked Experiment, Modeling & Simulation





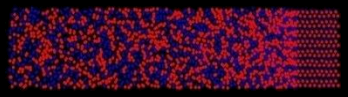
Ignition & Combustion/Propellants
- Chemical Mechanisms
- Plasma Ignition
- Kinetic Modeling

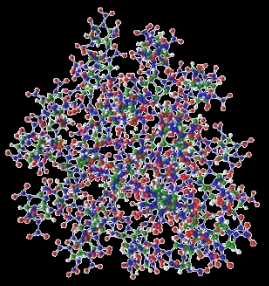
Propulsion Modeling/Guns & Rockets
- CFD NGEN3 & NSRG2
- Interior Ballistics, Simulator

Enhanced Blast Explosives
- Modeling
- Experiment/Diagnostics

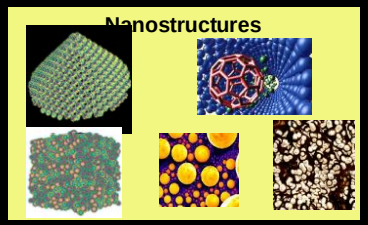
Detonation Modeling & Experiment
- Detonation
- Vulnerability
- Cook-off
- Sensitivity

Nano-Engineered Energetic Materials

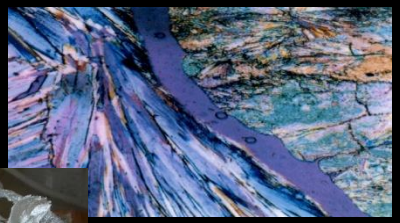


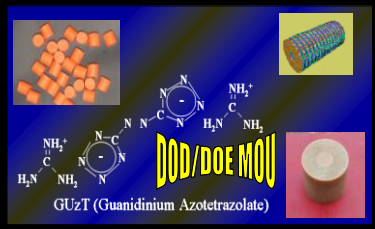


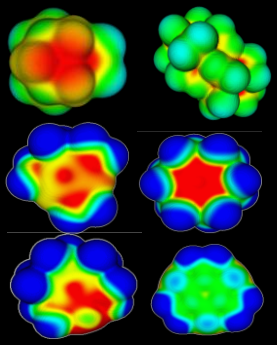
Molecular Dynamics & Molecular Simulation
- Energetic Polymers
- Gun/Rocket Propellants
- Mechanical Properties
- Detonation
- Burn Rate Prediction



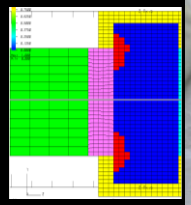
Reactive Monte Carlo
- Detonation Properties





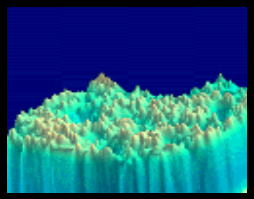


Quantum Mechanical
- Explosive Crystal
- Heats of Formation
- Density
- Sensitivity
- Rate Constants


Mechanical Properties
- Fracture - Experiment & Modeling
- Gas-Surface Interactions

Novel Propellant & Explosives



Thermochemical Modeling
- Heat Transfer
- Wear & Erosion

Design Tools for Energetics

Wise (old) Wizard Peering Over the Energetic Materials "alley of . eath" at the Synthesis Workshop

"Accelerating the transition of new energetic materials technologies into systems and products will be crucial to the Department of Defense's development of a lighter, more flexible fighting force"

Final Product

Scale-Up

Characterize

Yields

Performance

Quantities

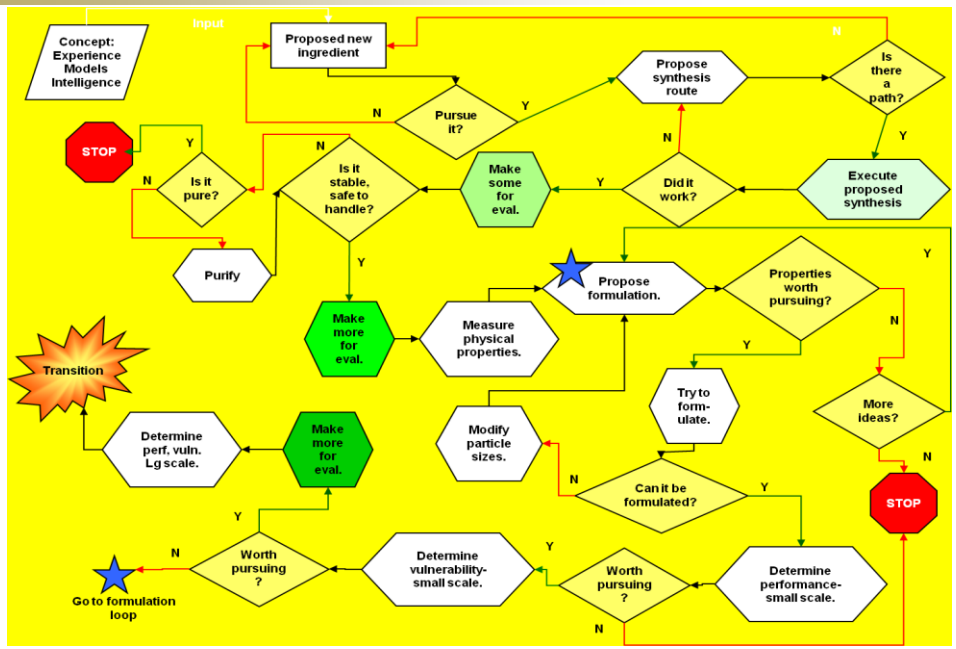
Sensitivity

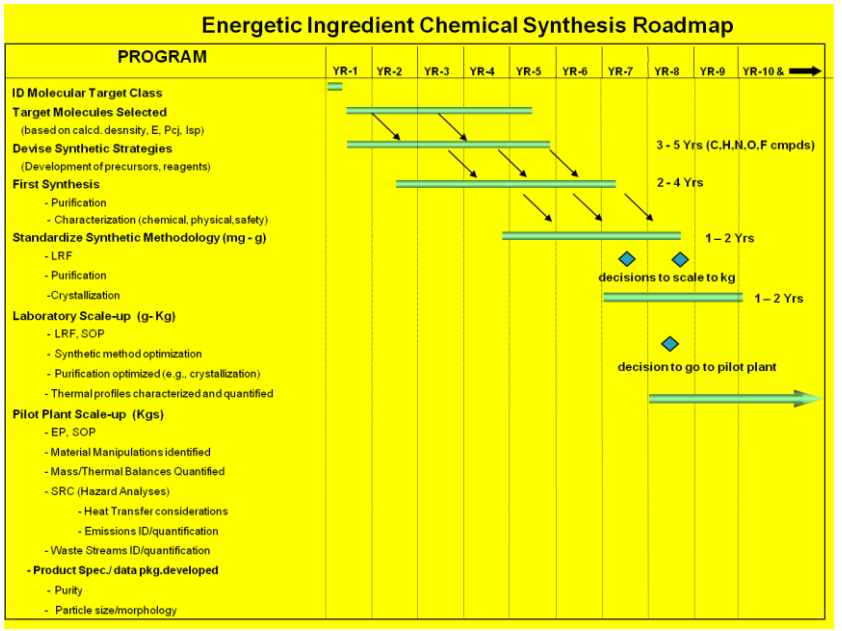
Routes

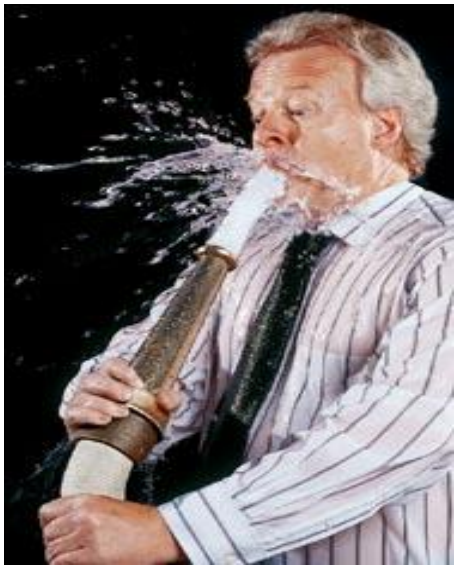
New Idea

Current long transition times-ten years or more are now typical and attributed to the complexity of the process.

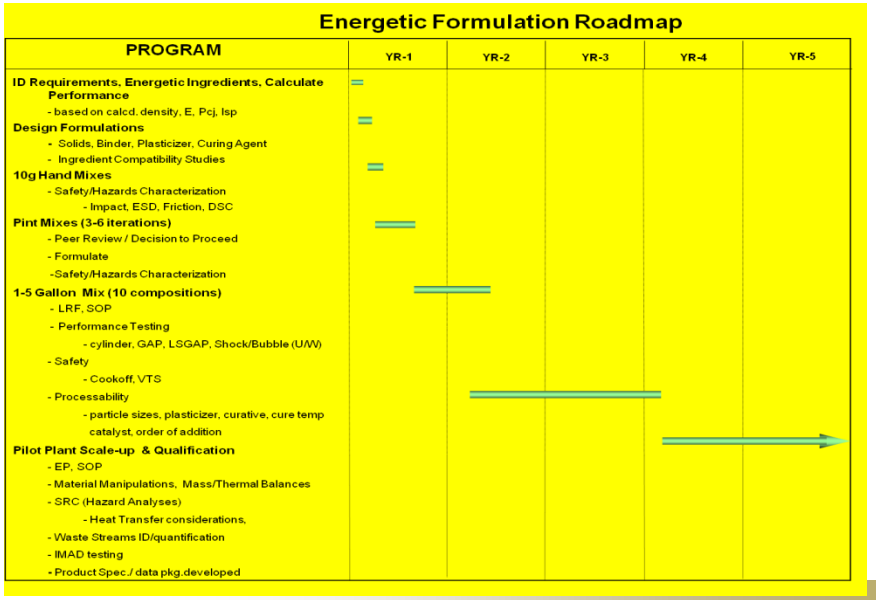
A Complex and Time Consuming Process







…there must be a simpler method?



Defense High Performance Computing

Insensitive Energetic Materials Formulations by Design

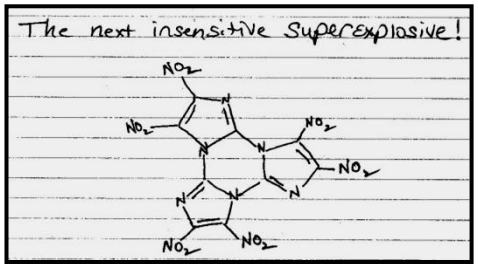
- High-Performance Computing (HPC):
  - » Delivers world-class, high-end, high performance computational capability to the DoD's science and technology (S&T) communities in advanced energetic materials (EM) research
  - » Is a critical enabler required in the study of advanced EM
  - » Facilitates the rapid application of advanced EM technology into superior warfighting capabilities
  - » Will provide a world class capability, within the DoD, and strengthened national prominence and preeminence by advancing critical EM technologies
  - » Worldwide research is accelerating

High Performance Computing is the Critical Factor Providing the Competitive Edge in Energetic Materials Research & Development

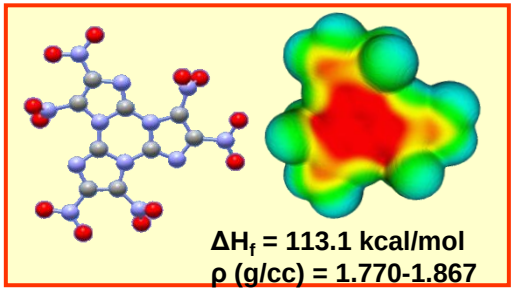
We can do this now: Smart Design of Energetic Ingredients

- **Purpose: Develop computational tools to predict the properties of EM to guide ingredient of synthesis**
- **Accomplishments:**
  - **Computational tools to predict performance, sensitivity, and environmental properties of energetic materials**
  - **Developed visual screening tool to assess sensitivity to impact using quantum mechanic information**
  - **Utilized condensed phase quantum and mechanical modeling methods to predict more dynamic and complex properties**
- **Impact: Reduce cost and expedite the development of advanced green energetic materials for Future Force green insensitive munitions**

Designer sends cartoon of candidate



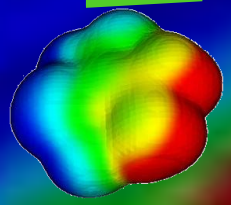
Application of theoretical chemistry tools



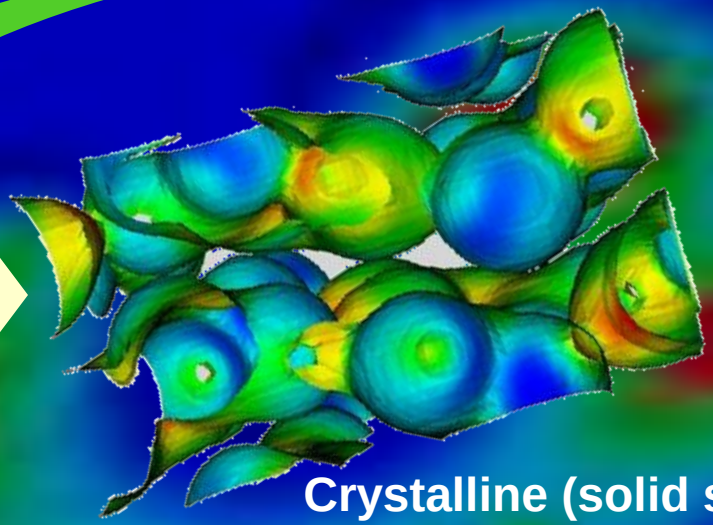
Predicted weapon performance

		Candidate
$\Delta H_{f(s)}$	Impetus (J/g):	1273
	Flame Temp (K):	4646
$\Delta H_{f(s)}$, ρ	Detonation Velocity (km/s):	8.5-8.8
	Detonation Pressure (GPa):	31.1-35
	Heat of Detonation (kJ/cc):	9-9.7

A Priori Predictions



Notional
New Energetics



Crystalline (solid state)

Properties Predictions:

- Structure
- Density
- Heats of Formation
- Heat of Detonation
- Sensitivity
- Toxicity

Toxicity & Fate/Transport

Use standard theoretical chemical approaches to

1. Screen proposed materials—eliminate poor candidates before expending resources on synthesis, formulation and tests
2. Identify and understand the individual fundamental chemical and physical steps that control the conversion of the material to final products

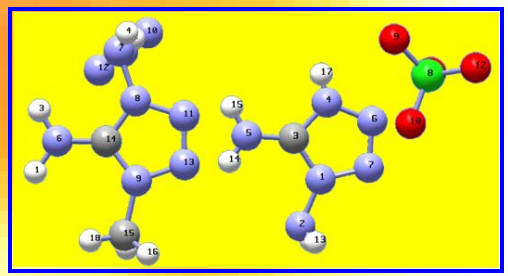
Quantitative Structure Property /Activity Relationships (QSPR/QSAR)

Predictive methodology using models based on statistical correlations between molecular properties and macroscopic behavior.

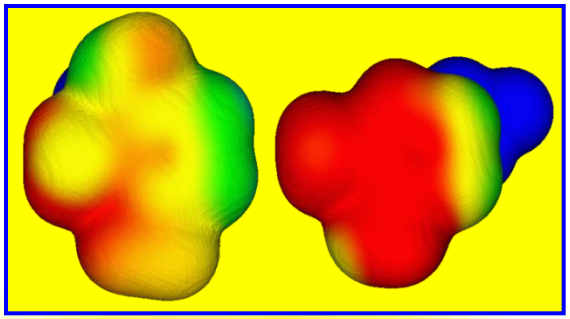
Smart & Agile Development of Novel Energetics From Quantum Mechanics to Quantities

RDECOM

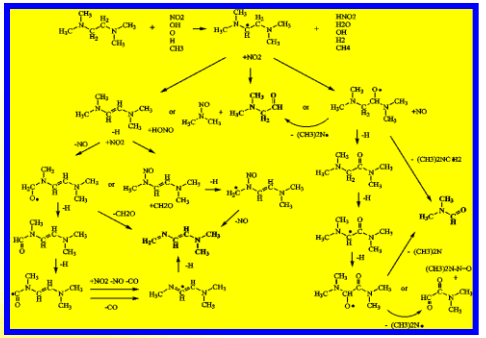
Design



Predict Properties



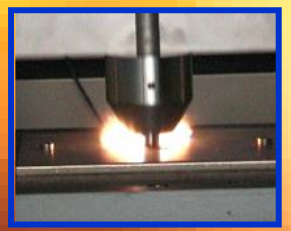
Develop Synthetic Routes



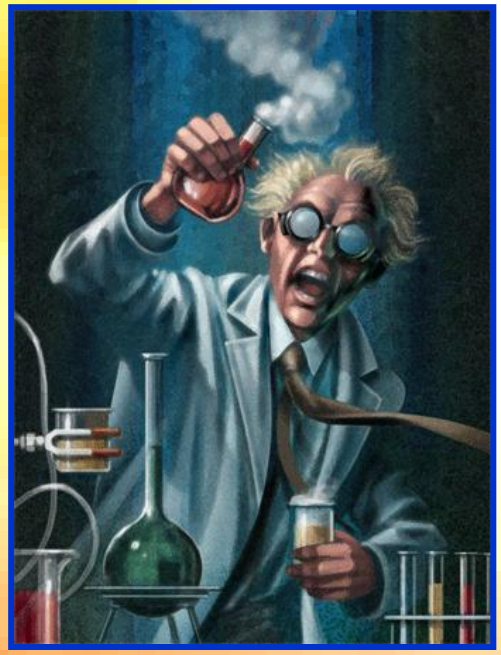
Performance Test

Formulate & Process

Characterize



Synthesize



Energetic Materials Science

Strategy

"Energetics" as a Material Science

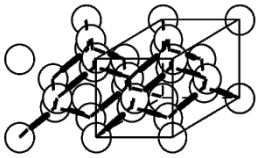
Decision Makers

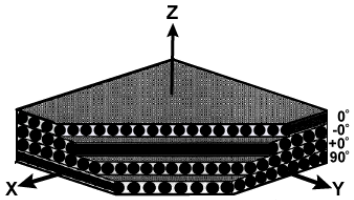
"..your new molecule has 10% greater energy than CL20, its %8 more dense, its green and looks insensitive, it cost twice as much but will be cheaper when a lot is produced later…what does this all mean…?"

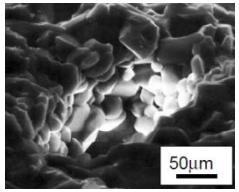
Energetic Materials Science

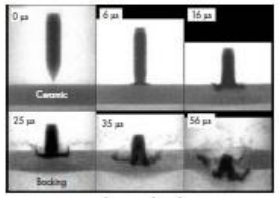
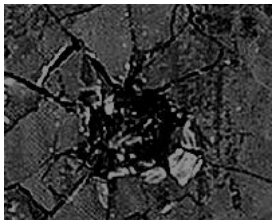
- Intent - to shape the direction of energetic materials research to achieve objectives that are materials-centric (formulation) and not ingredient-centric
  - Ingredients -> formulations -> materials -> engineered applications
  - Successful transitions to users are materials, not ingredients
- Elevate energetics to a materials science – "Energetic Materials Science"
  - Understand the connections between the underlying ingredients and structure of the energetic material, its properties, how processing and building changes it, and what the material can do - its performance, sensitivity, stability, etc.
- For decades the energetic materials community has focused on ingredient development, and research focused on the properties and behavior of ingredients
- But understanding ingredients alone and at high fidelity does not ensure the transition to a formulation (a complex material)
  - This has been a bottle neck that must be overcome
- Energetic materials must be viewed as a "materials science" – which requires understanding energetics at multiple length and time scales – atomistic, molecular, micro, and meso – as a material
  - Complex material with energetic ingredients, crystals, particles, binder, etc
  - Processing, mixing, fabrication, production of materials
- Develop the fundamental and applied knowledge to optimize the full range of properties of energetics as a complex material

Material Science Analogy → Products





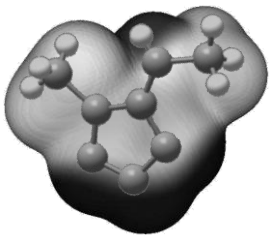


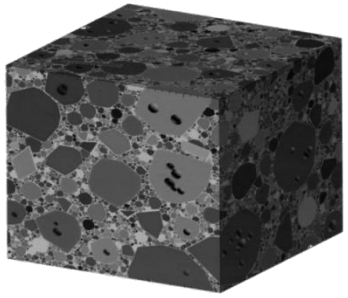



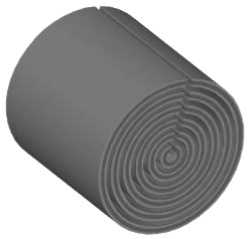
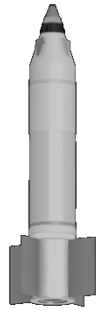
CERAMIC MATERIAL

New Structure → Synthesize → Formulate → Performance Test → New Material → New Product

ENERGETC MATERIAL





Translate the features of the new molecule to the attributes that will be enabled by its use in the final product(s).

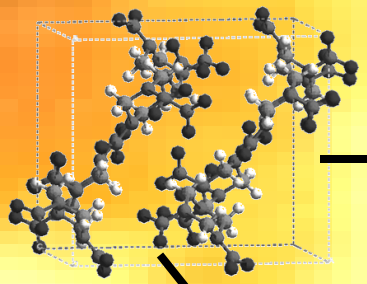
The material scientists are very good at doing this!

- **One munition can replace several**
- **Twice the lethal radius**
- **Munition passes IM tests**
- **No adverse environmental effects**
- **Extended use lifetime**

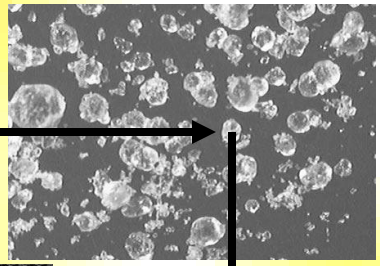
Multi-Scale M&S of Energetic Materials
Quantum → Continuum

Capture Accurate Physical & Chemical Descriptions

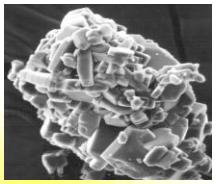
Molecules



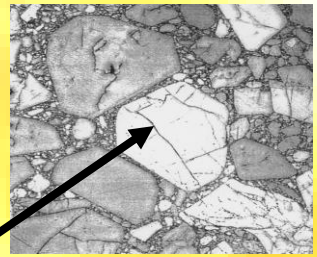
Crystals



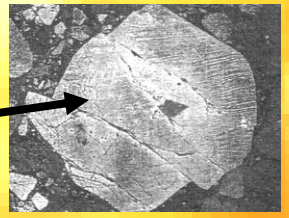
Crystal-Binder



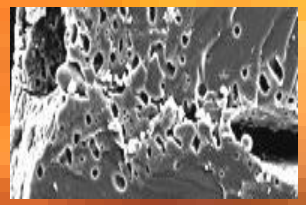
Cracking



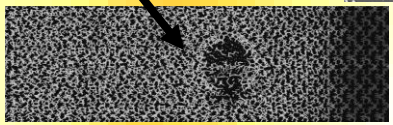
Shearing



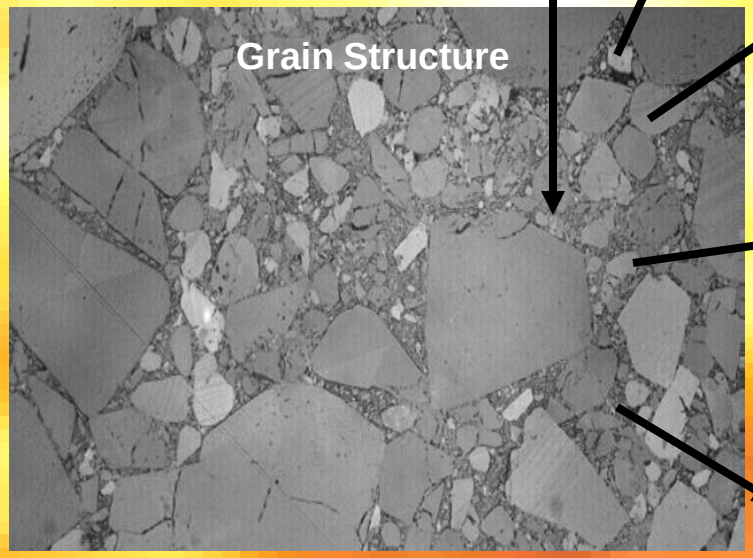
Decomposing
Initiating & Reacting



Defects

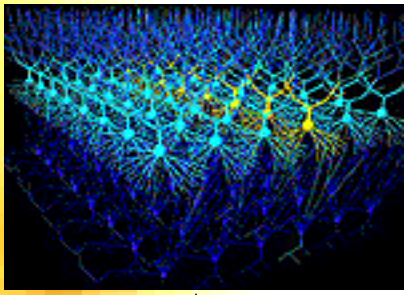


Mechanical Properties

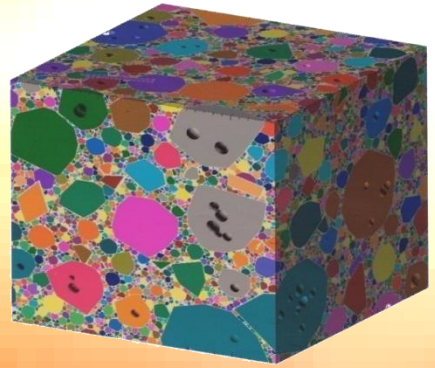


Processing Performance Sensitivity
Stability Lifecycle

Materials Engineered
for Munitions Applications

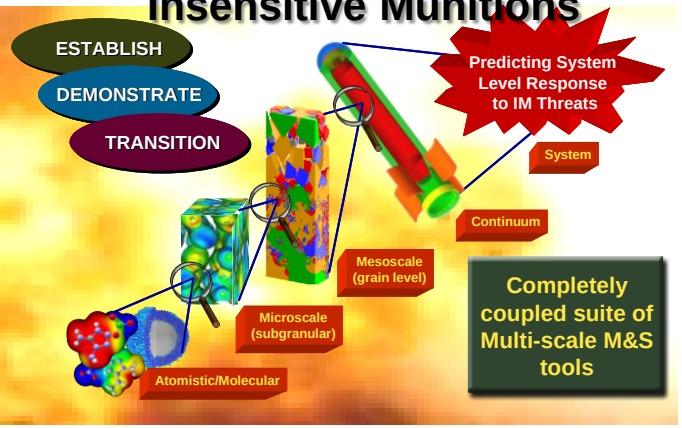


Robust Predictive Model of Energetic
Materials Properties & Behavior

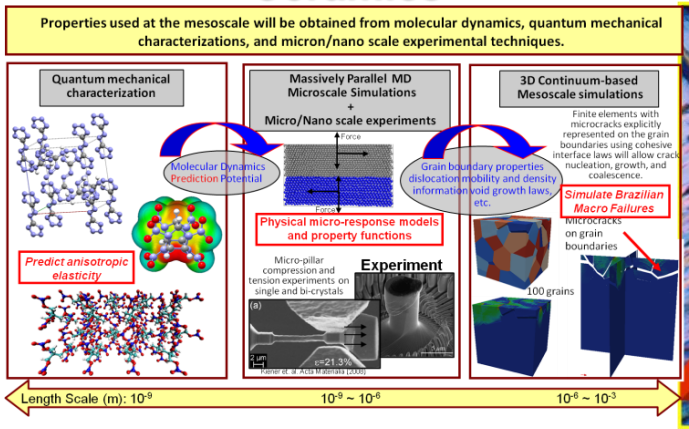


Did anyone say Multi-Scale Modeling & Simulation?

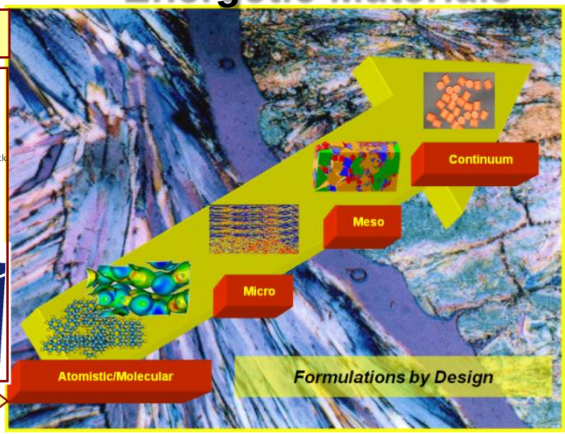
Insensitive Munitions



Ceramics

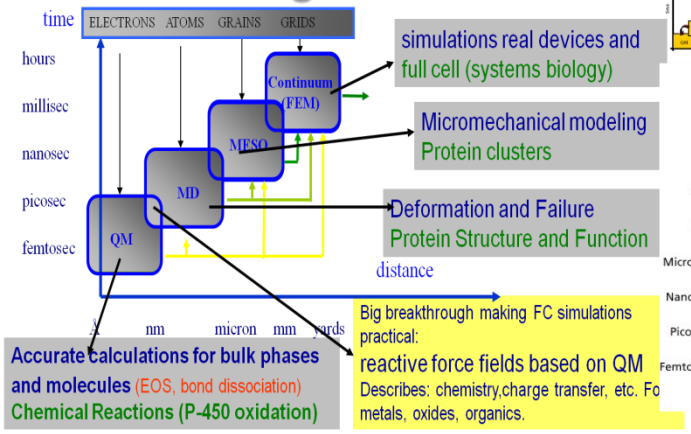


Energetic Materials

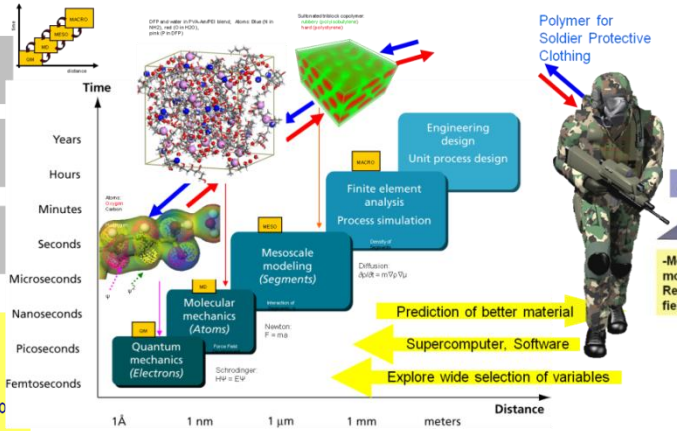


From the bottom up….. *ab-initio* science that will enable the four dimensional (4-D) spatial & temporal theoretical portrayal of large-scale, complex materials of interest.

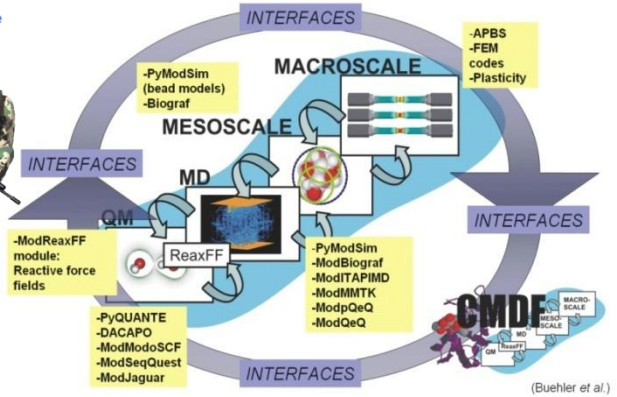
Biological Materials



Multi-Functional Materials

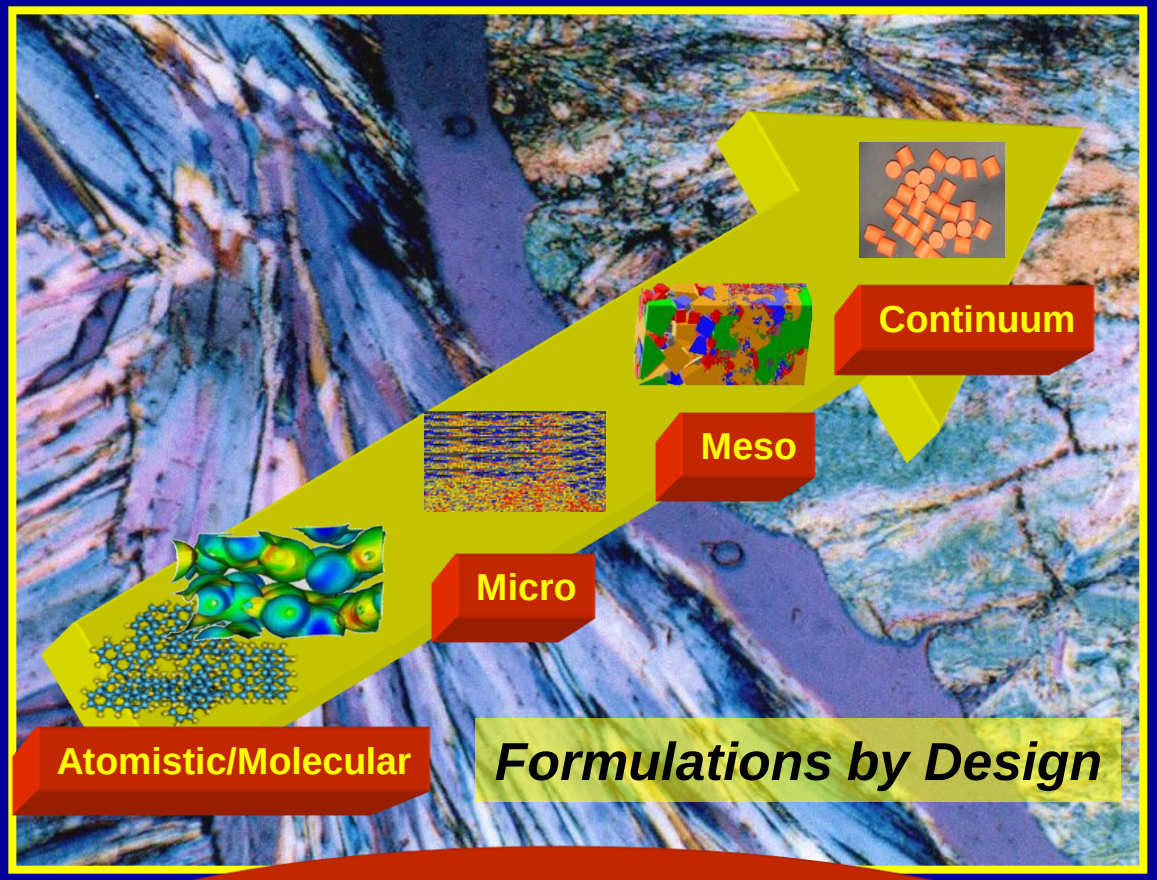


Electronic Materials



How to do this is the Great Debate!

Multi-Scale Modeling:
Not Just Ingredients – the Whole Material



Advances in improving explosive performance and the design of new energetics will follow with improved understanding of the thermal, mechanical, and chemical processes at the atomistic, microscopic and mesoscopic scales

Different time and length scales require different theoretical models

Multi-scale Modeling links time and spatial regimes

Goal: Utilization of Computational tools to design novel energetic materials formulations with optimized properties

A new effort to help in Energetic Materials Science Quests: High-Performance Computing Institute for Multi-Scale Reactive Modeling and Simulation of Insensitive Munitions

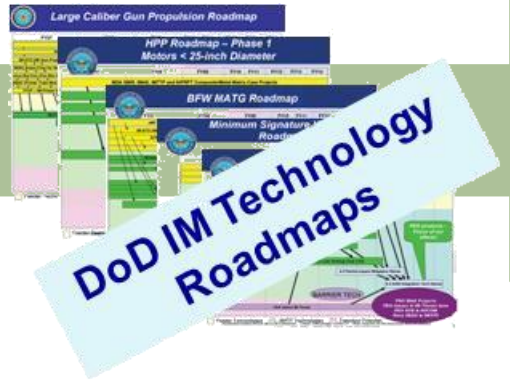
Six-Year Program

User Requirements

Gaps & Shortfalls

PEO/PM Priorities

Joint Service IM Technology Program Roadmaps

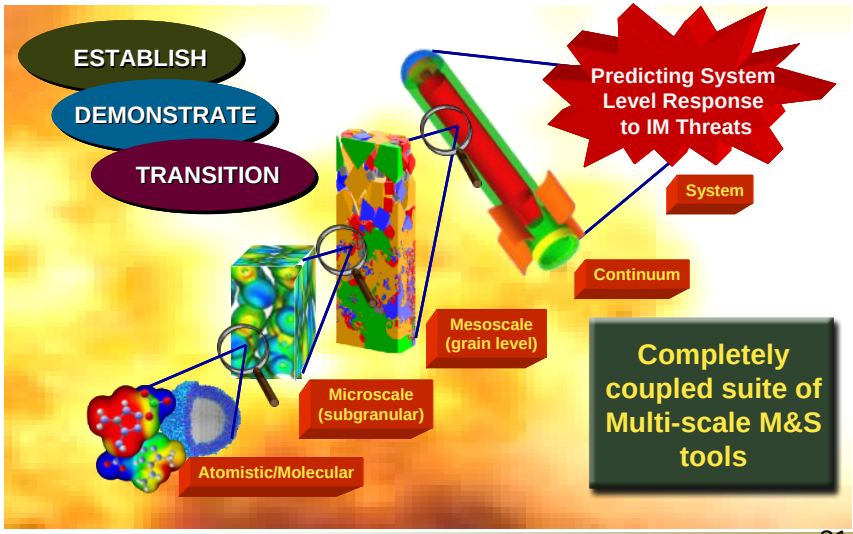


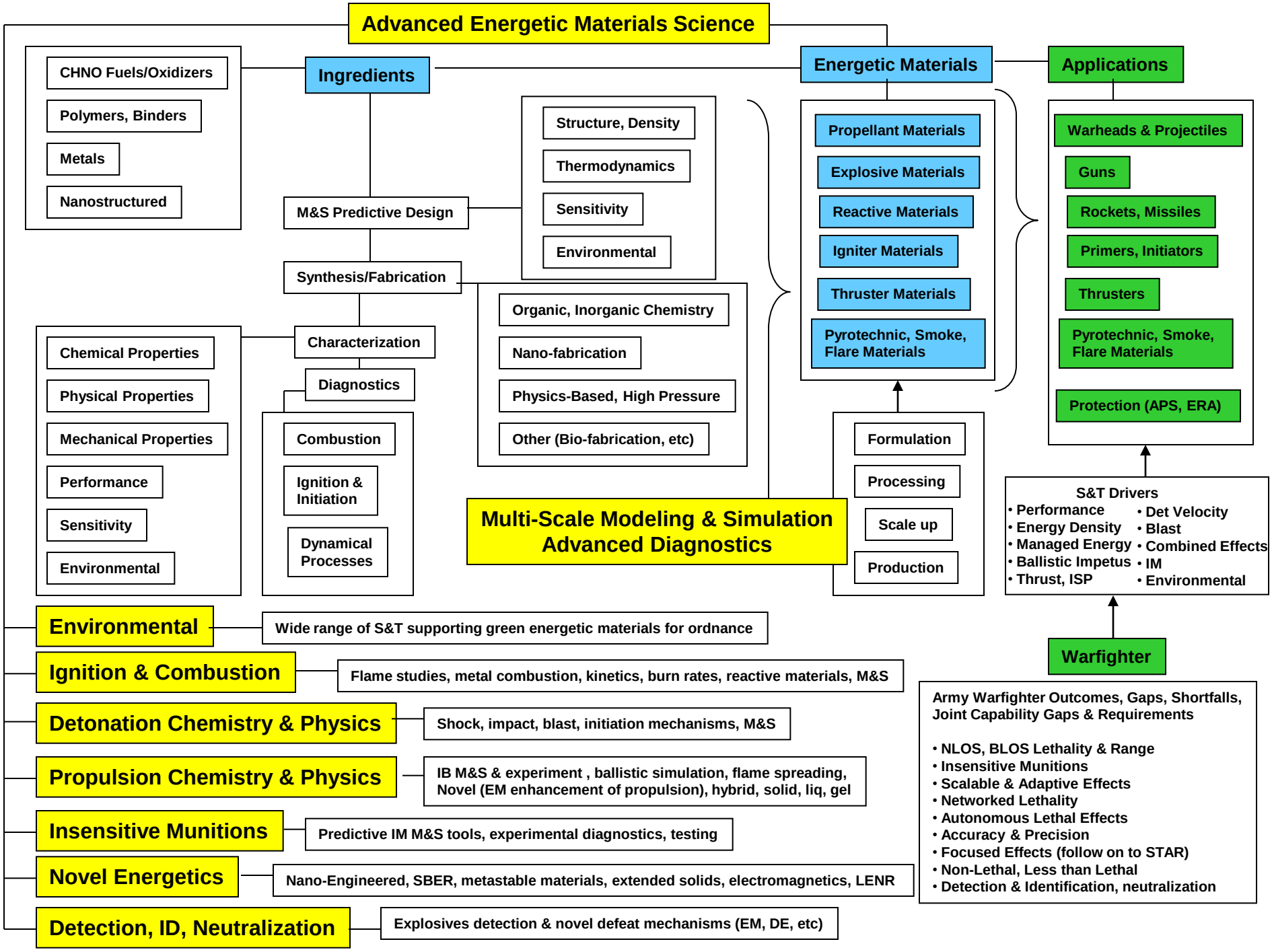
PRODUCTS

HPC Modernization Program

Institute will *revolutionize* M&S in munition design process

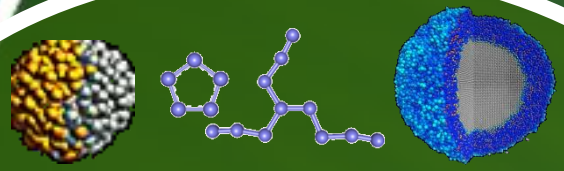
- Multiscale capability, incorporating fundamental physics/chemistry
- Reduction of empiricism
- Faster Design and Implementation
- Reduced risk, cost and time
- Extrapolation to novel, potentially more capable designs




Advanced Energetic Materials Science
Ingredients
CHNO Fuels/Oxidizers
Polymers, Binders
Metals
Nanostructured
M&S Predictive Design
Structure, Density
Thermodynamics
Sensitivity
Environmental
Synthesis/Fabrication
Organic, Inorganic Chemistry
Nano-fabrication
Physics-Based, High Pressure
Other (Bio-fabrication, etc)
Characterization
Chemical Properties
Physical Properties
Mechanical Properties
Performance
Sensitivity
Environmental
Diagnostics
Combustion
Ignition & Initiation
Dynamical Processes
Energetic Materials
Propellant Materials
Explosive Materials
Reactive Materials
Igniter Materials
Thruster Materials
Pyrotechnic, Smoke, Flare Materials
Applications
Warheads & Projectiles
Guns
Rockets, Missiles
Primers, Initiators
Thrusters
Pyrotechnic, Smoke, Flare Materials
Protection (APS, ERA)
Formulation
Processing
Scale up
Production
Multi-Scale Modeling & Simulation
Advanced Diagnostics
S&T Drivers
• Performance
• Energy Density
• Managed Energy
• Ballistic Impetus
• Thrust, ISP
• Det Velocity
• Blast
• Combined Effects
• IM
• Environmental
Warfighter
Army Warfighter Outcomes, Gaps, Shortfalls, Joint Capability Gaps & Requirements
• NLOS, BLOS Lethality & Range
• Insensitive Munitions
• Scalable & Adaptive Effects
• Networked Lethality
• Autonomous Lethal Effects
• Accuracy & Precision
• Focused Effects (follow on to STAR)
• Non-Lethal, Less than Lethal
• Detection & Identification, neutralization
Environmental
Wide range of S&T supporting green energetic materials for ordnance
Ignition & Combustion
Flame studies, metal combustion, kinetics, burn rates, reactive materials, M&S
Detonation Chemistry & Physics
Shock, impact, blast, initiation mechanisms, M&S
Propulsion Chemistry & Physics
IB M&S & experiment , ballistic simulation, flame spreading, Novel (EM enhancement of propulsion), hybrid, solid, liq, gel
Insensitive Munitions
Predictive IM M&S tools, experimental diagnostics, testing
Novel Energetics
Nano-Engineered, SBER, metastable materials, extended solids, electromagnetics, LENR
Detection, ID, Neutralization
Explosives detection & novel defeat mechanisms (EM, DE, etc)

US ARMY RDECOM

Put Overwhelming Firepower in the Hands of the War Fighter



- Meta-Stable Atoms, Molecules
- Nano-Engineered Energetics
- Strained Energy Materials
- Novel Metals, Reactive Structures

We Have This
Current Explosives
TNT, RDX, CL20

We Don't Have This
Disruptive Energetics
THE QUEST

We Have This
Nuclear
Sub-Atomic Processes
Nuclear Spin Isomer $^{178}Hf^{m2}$
Nuclear Fission ^{235}U
Nuclear Fusion D-T

We Don't Have This
Anti-Matter Annihilation e^- / e^+

10^3 10^4 10^5 10^6 10^7 10^8 10^9 10^{10} 10^{11} 10^{12} 10^{13} 10^{14} 10^{15} J/g

Energy Density Scale

Soldier as a System
Overwhelming Firepower in the Hands of the Warfighter

The Future of Advanced Energetic Materials? Predicting the Future from Expert Perspectives

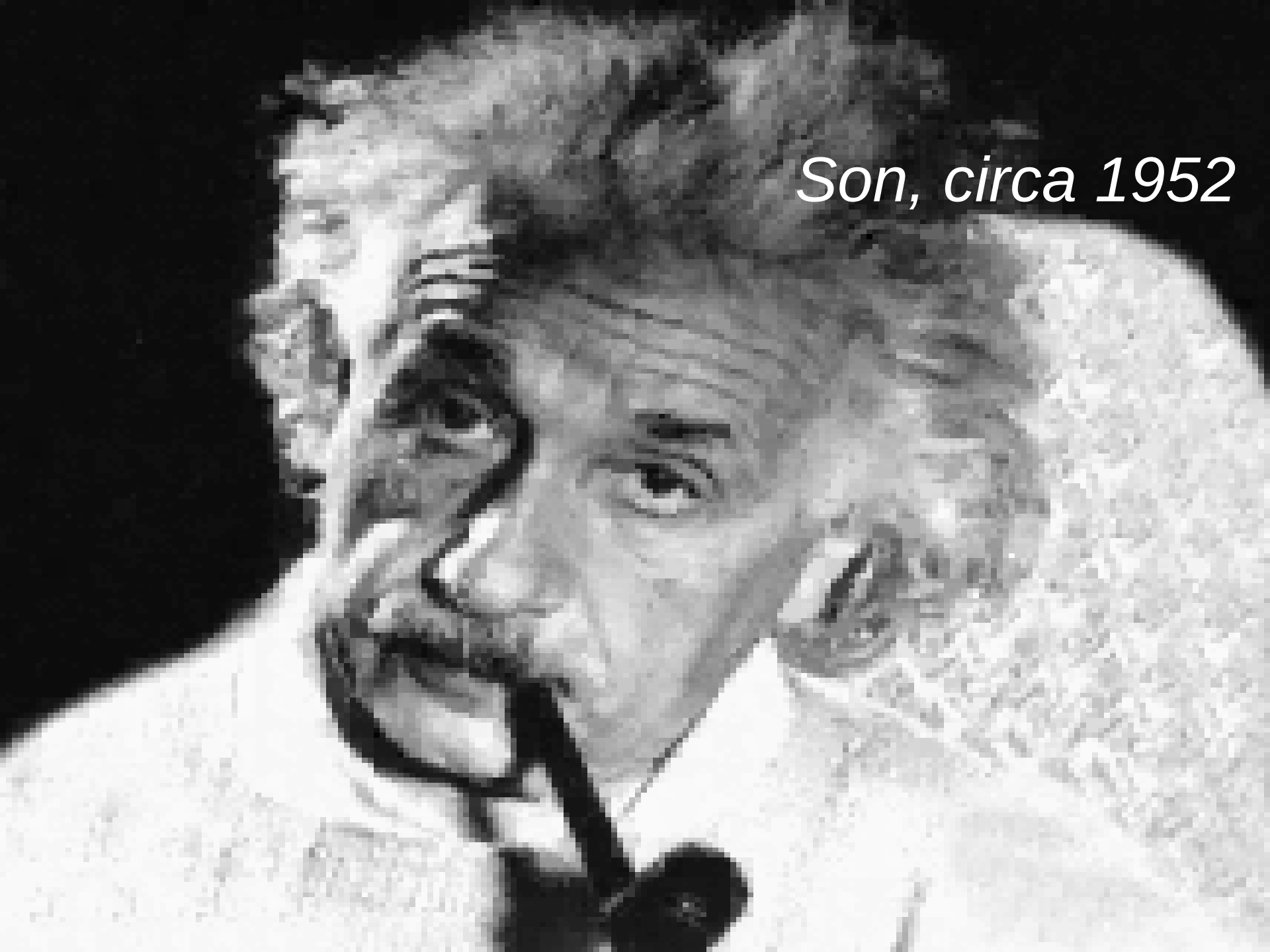
It's tough to make predictions, especially about the future. Some famous technology predictions include:

- ***"Heavier-than-air flying machines are impossible."***
  - ***Lord Kelvin, 1895***
- ***"Airplanes are ...of no military value."***
  - ***Marshal Ferdinand Foch, 1911***
- ***"Who ... wants to hear actors talk ?"***
  - ***H. M. Warner, 1927***
- ***"... (T)here is world market for maybe five computers."***
  - ***T. Watson, IBM Chairman, 1943***
- ***"640k (RAM) ought to be enough for anybody."***
  - ***Bill Gates, 1981***

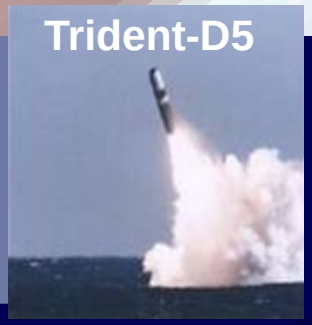
Father's Prediction

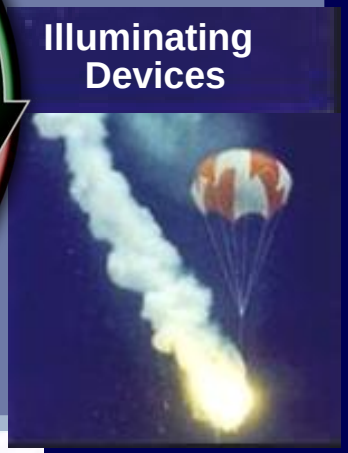
e.d.…."you'll never amount to anything, all you care about is shooting guns and catching rats…"

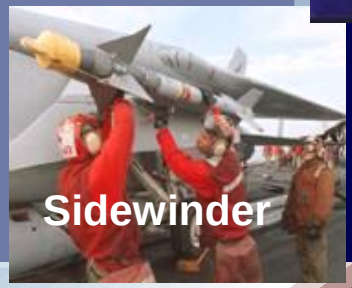
Father's admonition to his son, circa 1885

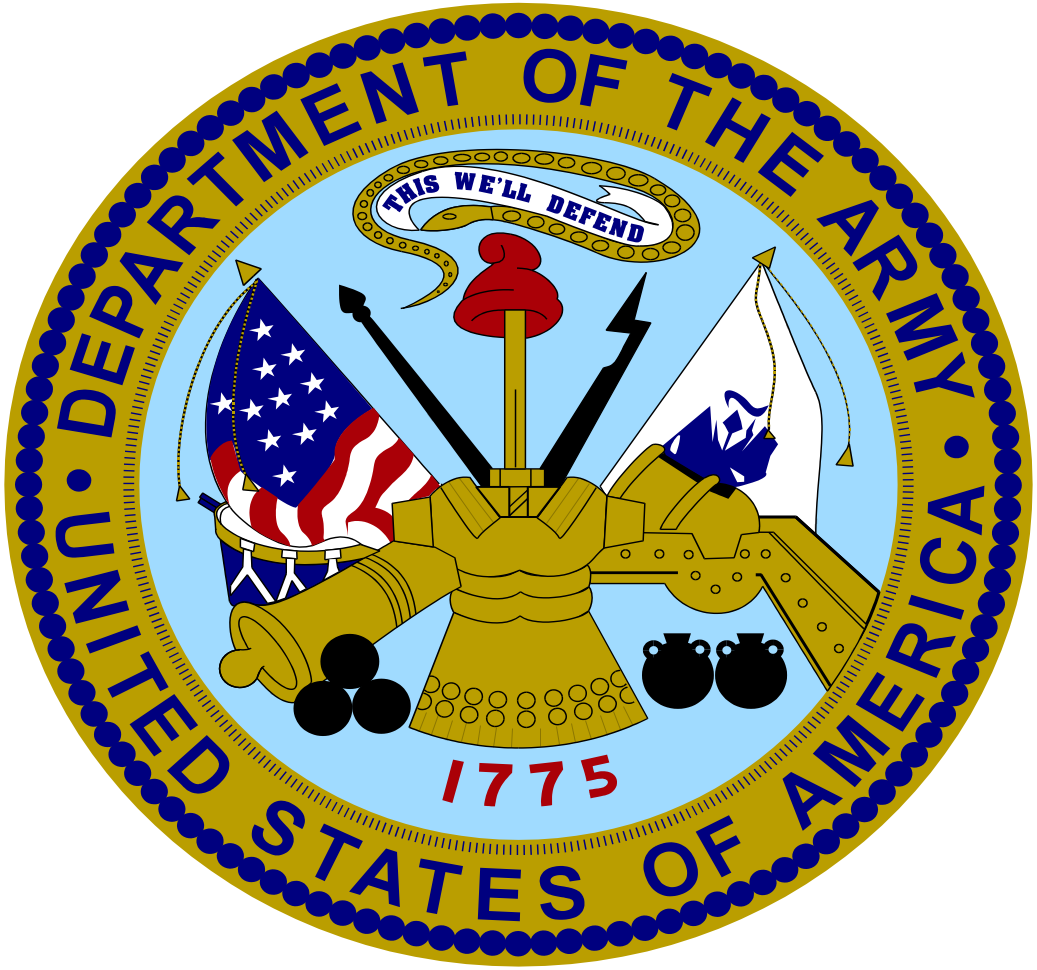

Son, circa 1952

Prediction: New Energetic Materials will be an Enduring Need for the Future Weapons Enterprise








DEPARTMENT OF THE ARMY
UNITED STATES OF AMERICA
THIS WE'LL DEFEND
1775