Disruptive Energetics- Fundamental Science for the Future

Dr. Jennifer A. Ciezak-Jenkins

Wednesday April 27, 2016

U.S. ARMY RDECOM®

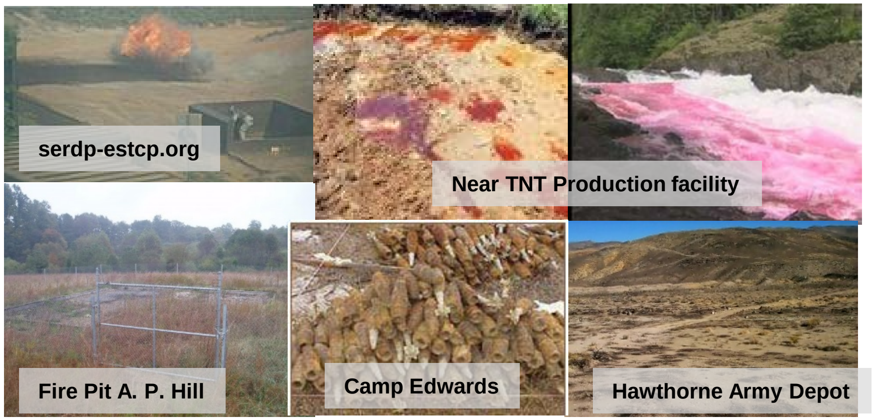
Drivers for Energetics

ARL

Insensitive Munitions

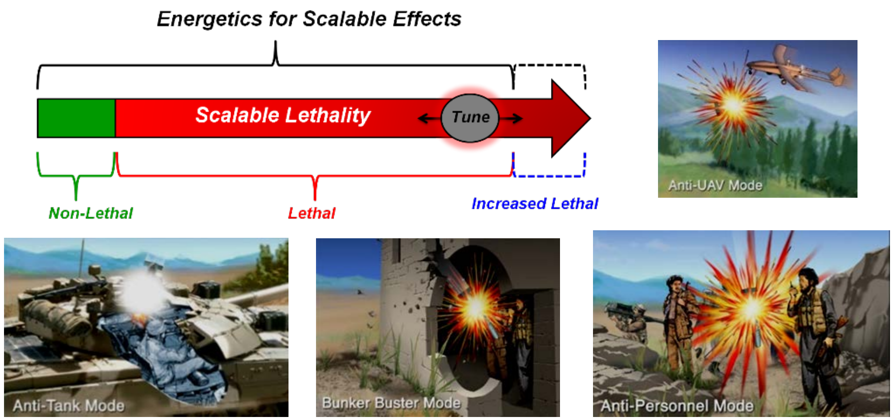
Warfighter Survivability

Green Insensitive, High-Performance



Swarming Multi-Agent Systems & Micro Munitions

Scalable & Multipurpose Effects



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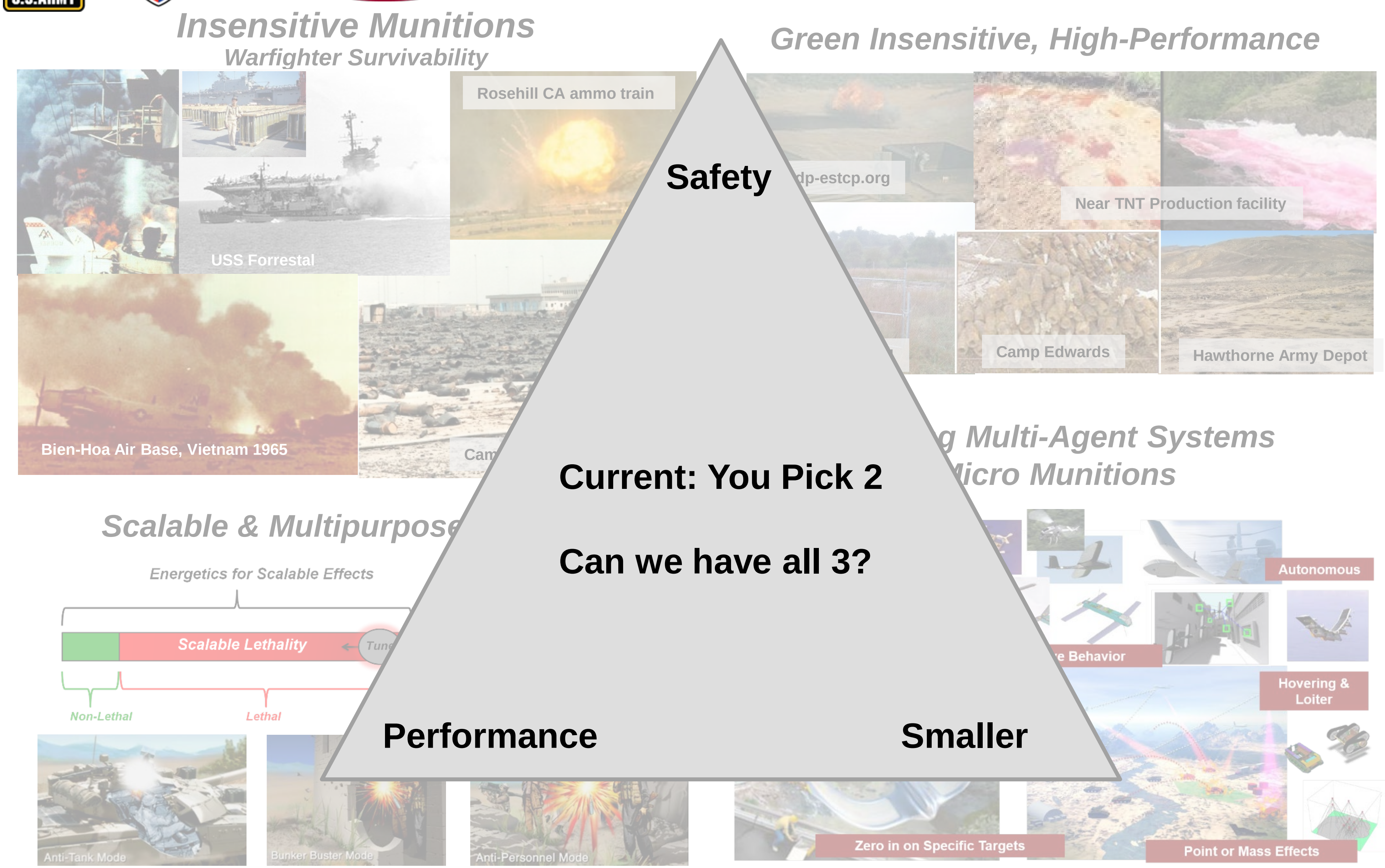
Drivers for Energetics

ARL



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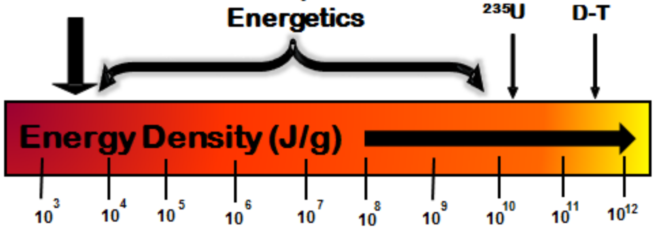
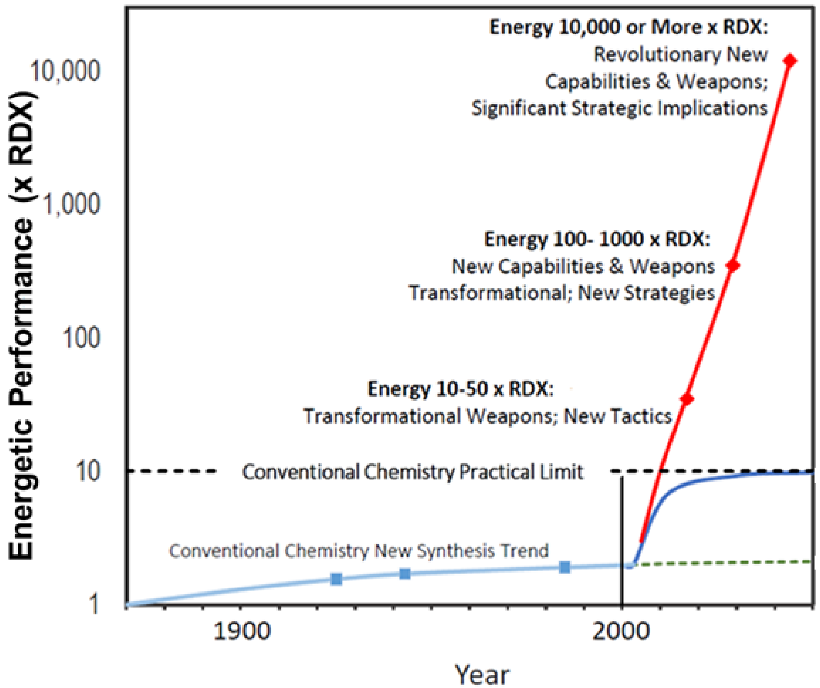
State of Energetics

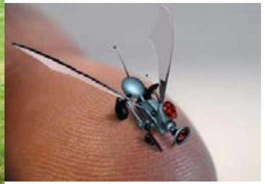
ARL

Challenge : To accelerate the discovery and development of game-changing capability which will enable transformational lethality for the Army of 2040

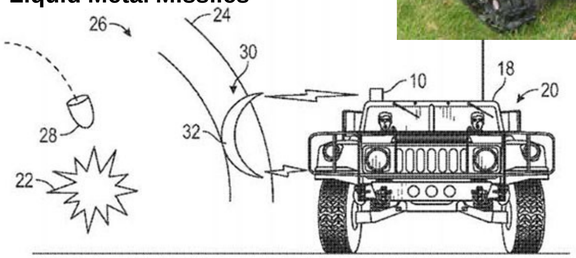




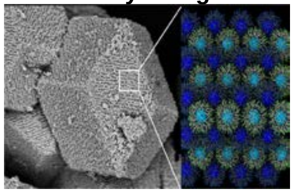
Small Combat UGV

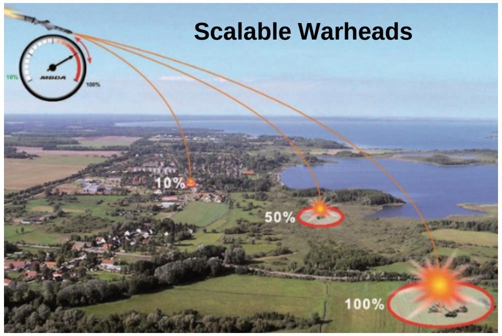


Liquid Metal Missiles



Materials by Design





Energetics for Weapons
Substantial Improvements can be Achieved

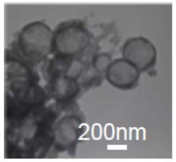
Pathways for moving beyond SOA

IMPROVING EXISTING CAPABILITIES – *NEAR TERM*:

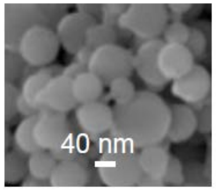
(LOW RISK/LOW-MED PAYOFF)

- Nanoenergetics
- Co-crystals etc
- Lots of other ideas out there in the literature

CL-20/NC Cryogel



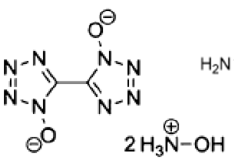
nAl



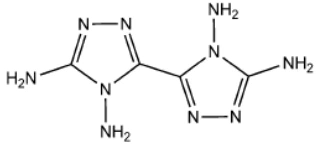
SYNTHESIS OF NEW MATERIALS – *MID TERM*:

(MED RISK/ LOW-MED PAYOFF)

- Synthesize and characterize energetic materials for optimal tailorable performance
- Not much new under the sun
- Shortfall of energetic chemists worldwide



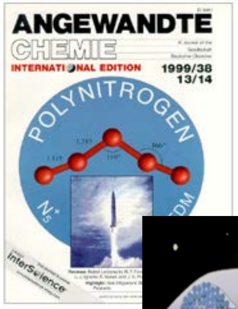
TKX-50

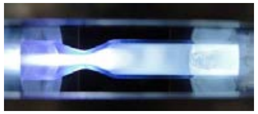


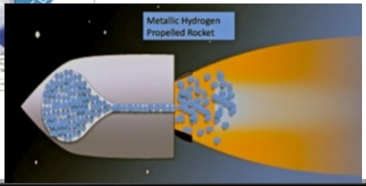
DISRUPTIVE APPROACHES - *FAR TERM*:

(HIGH RISK/HIGH PAYOFF)

- Materials with orders of magnitude of improvement
- Discovery and development of revolutionary energetic materials with properties radically superior to current capabilities.
- Research approach diverges towards innovative disruptive physics-based methods.







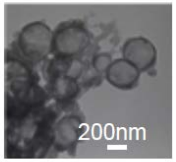
Pathways for moving beyond SOA

Improving Existing Capabilities – *Near Term*:

(Low Risk/Low-Med Payoff)

- Nanoenergetics
- Co-crystals etc
- Lots of other ideas out there in the literature

CL-20/NC Cryogel



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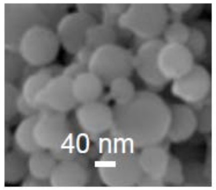
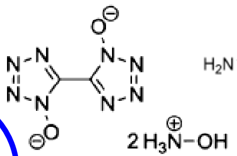


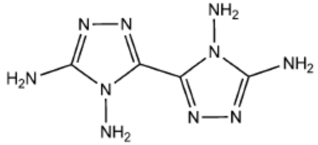
Synthesis of New Materials – *Mid Term*:

(Med Risk/ Low-Med Payoff)

- Synthesize and characterize energetic materials for optimal tailorable performance
- Not much new under the sun
- Shortfall of energetic chemists worldwide



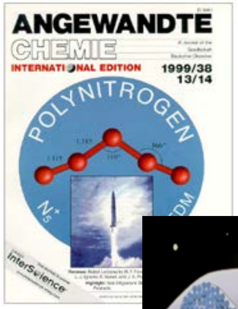
TKX-50

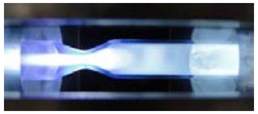


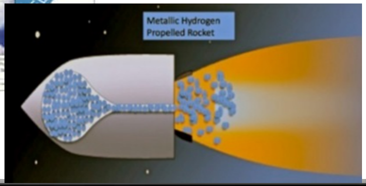
Disruptive Approaches - *Far Term*:

(High Risk/High Payoff)

- Materials with orders of magnitude of improvement
- Discovery and development of revolutionary energetic materials with properties radically superior to current capabilities.
- Research approach diverges towards innovative disruptive physics-based methods.

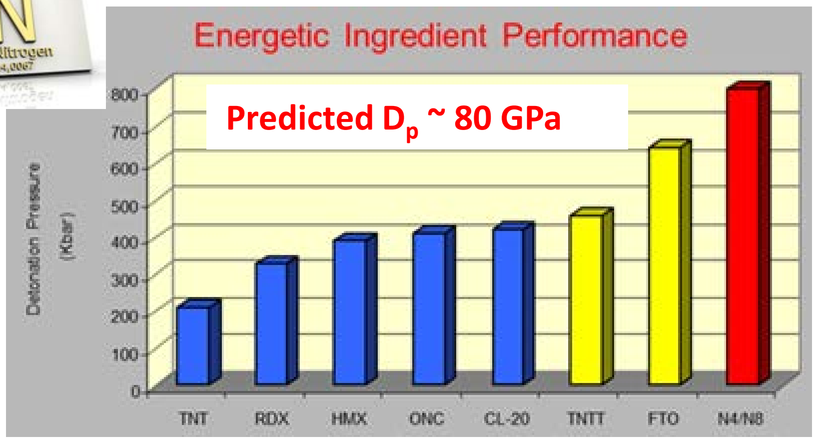


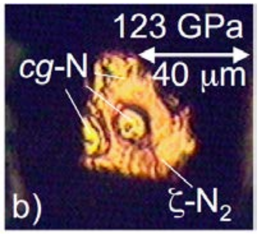


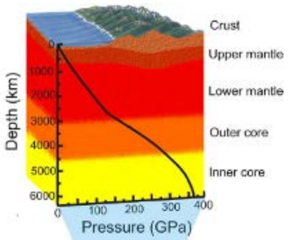


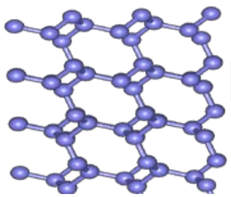
Polymeric Nitrogen – a bifunctional energetic/propulsive material?

The Interest as Energetic



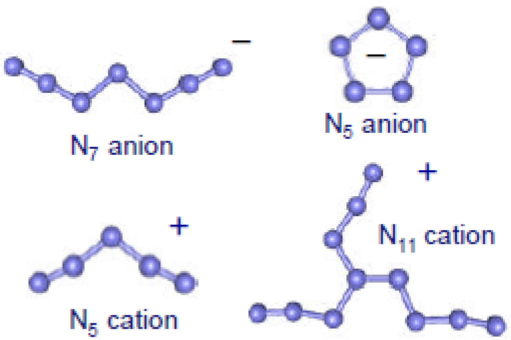






N≡N + ~800 kJ/mol

The Interest as Propellant



Predicted I_{sp} of 500 sec

The Challenge of Synthesis

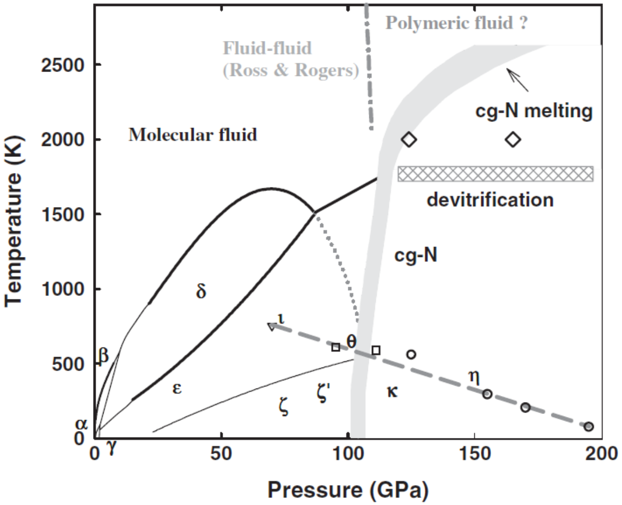
- ***Synthesis in 2004 near 120 GPa coupled with temperatures of 2000K***

Comparable to PT in lower mantle <u>~1800 miles</u> below surface

- ***Recovery to 50 GPa at RT***

1 GPa ≈ 10000atm

The Real Challenge remains <u>Stabilization</u>

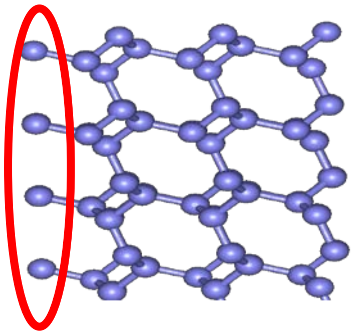


Goncharov et al. PRL (2008)

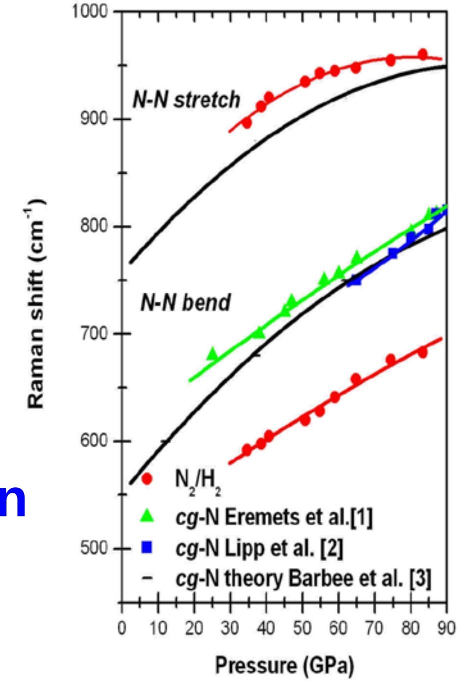
Stabilization of Polynitrogens- Via hydrogen doping

N_2/H_2 mixtures: A viable method for inducing metastability?

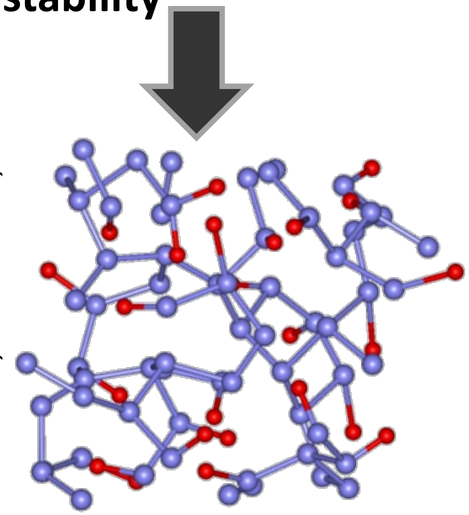
J.A. Ciezak et al. Proceeding SCCM 2009



6 GPa | 30 GPa | 80 GPa

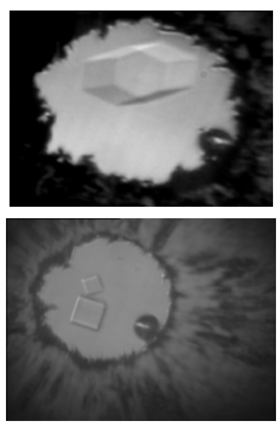


Passivation of terminal ends with hydrogen promotes stability

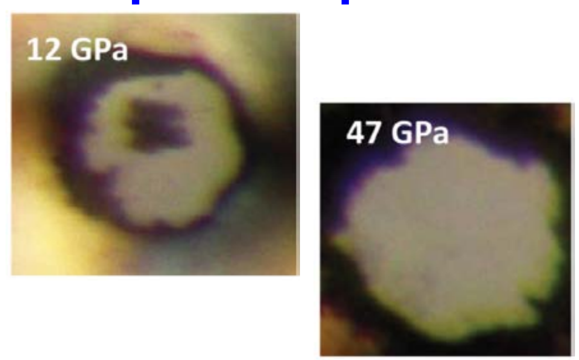


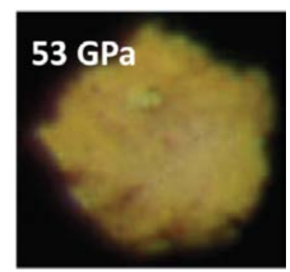
W.D. Mattson, Ph.D Thesis, 2003

More recent results have shown multiple new phases



Spaulding et al. Nature Comm., 5:5739 (2014)



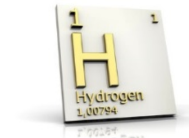


Goncharov et al. JCP 142 214308 (2015)

But still no recovery to date.

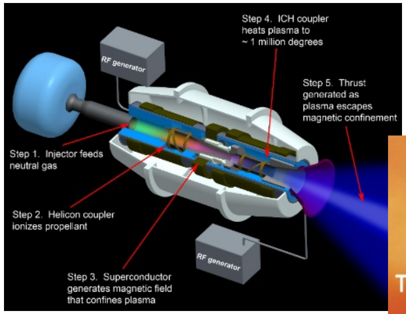
Metallic Hydrogen
Far term Propulsion Solutions

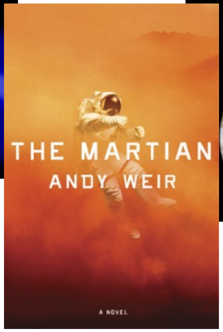
Some Remarkable Predicted Properties of Metallic Hydrogen

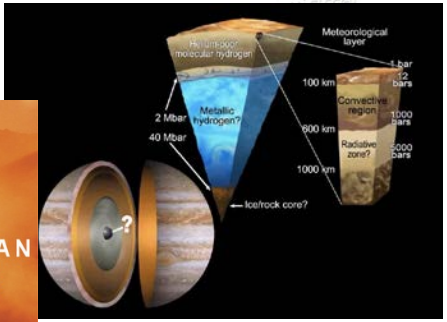


- ***Recombination of hydrogen atoms releases 216 MJ/kg***
- ***Hydrogen/Oxygen combustion in Shuttle 10 MJ/kg***
- ***Detonation of TNT 4.2 MJ/kg***
- ***Theoretical Specific Impulse – 1000-1700 s***
- ***Specific Impulse H_2/O_2 space shuttle – 460s***

Metallic Hydrogen Propelled Rockets



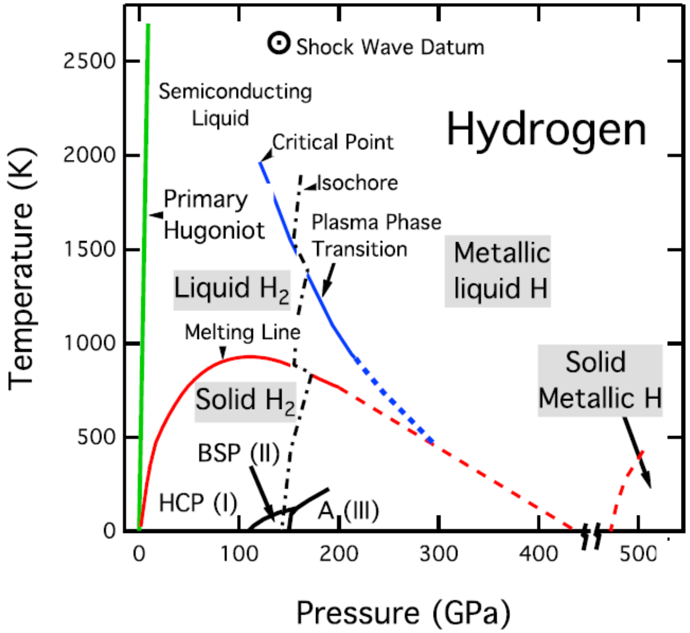




Proposed Reservoirs on Jupiter

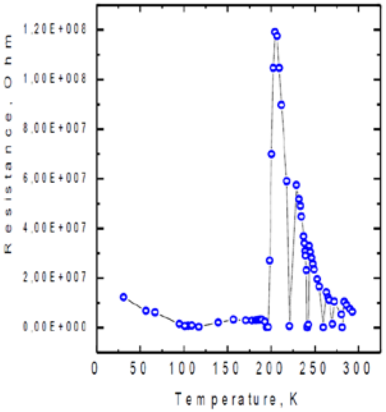
Phase Diagram of Hydrogen: Theory and Experiment

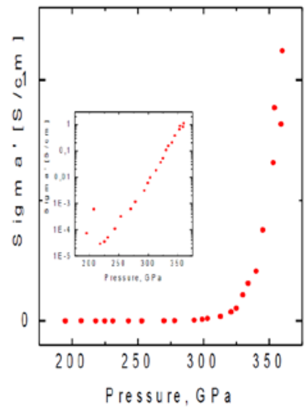
Silvera, PNAS, 107, 12743, 2010



Success in 2016 at 360 GPa and 200K?

Abrupt drop in Resistivity suggests Metallization





Eremets et al. submitted 2016

Intense Debate among researchers in field – Strong evidence still remains elusive!

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Modeling and Simulation- A vector for understanding complex experiments

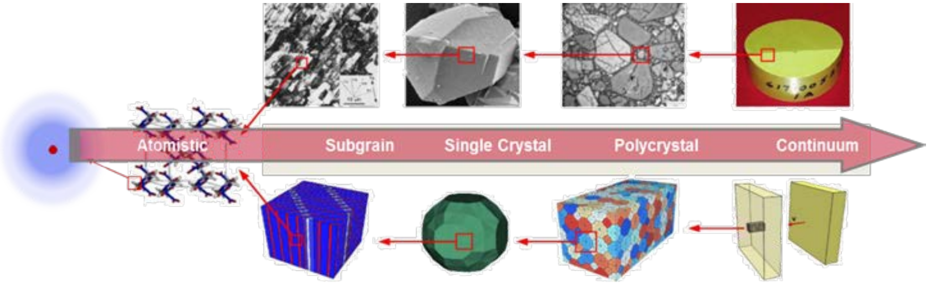
ARL

COMPUTATIONAL RESEARCH IN ENERGETICS

- Enable new energetics technologies
- Understand new ways to store and release energy
- Design energetic structures tailored for optimal performance

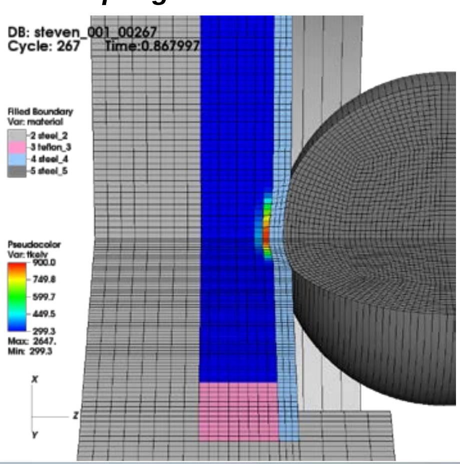
Virtual Design Computational Screening Toolkit

Multiscale Response of EM

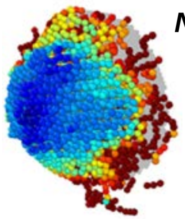


Shear Banding in RDX

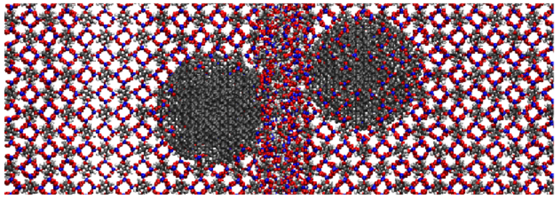
Coupling to continuum

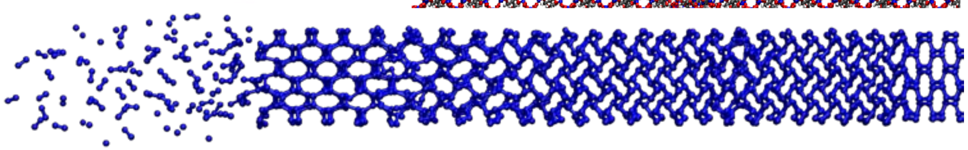


QM Simulations of Disruptive Energetic Materials under Shock

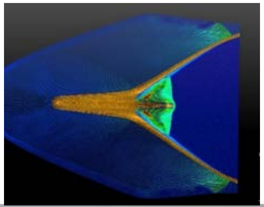


Nanomaterials

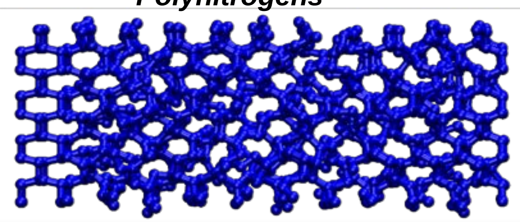




Initiation Mechanisms



Polynitrogens



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Getting more energy out of energetics – What is the most crucial excitation mechanism?

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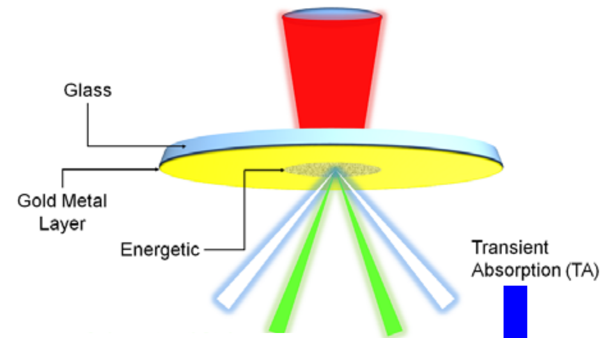
ULTRAFAST DYNAMICS OF ENERGETIC MATERIALS

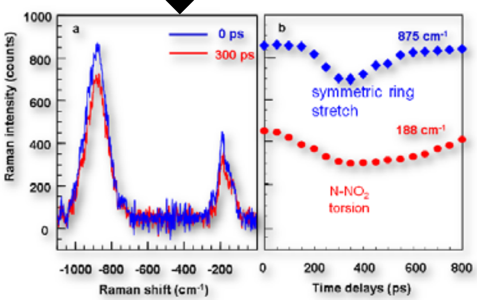
DEVELOP BETTER DETONATION MODELS AND UNDERSTAND HOW TO CONVERT STORED CHEMICAL ENERGY INTO MECHANICAL ENERGY

- Understand molecular response of energetic materials at very earliest times of initiation and detonation
- Understand energy flow processes from the initial dynamic stimuli through energetic initiation processes

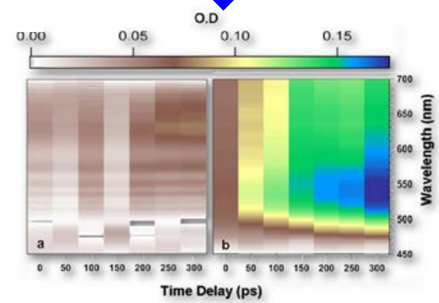
Indirect Laser Heating



Coherent Anti Stokes Raman (CARS)

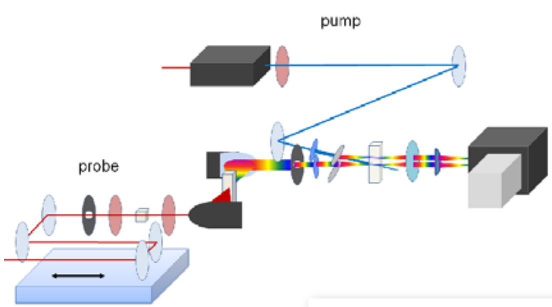


Observe chemical dynamics under influence of temp alone

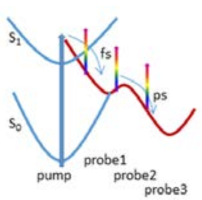


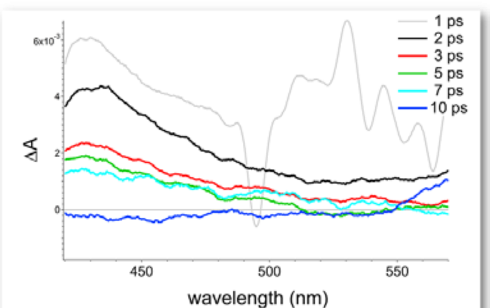
Observe electronic excitations due to temp

Optical Pumping of Excited State Dynamics

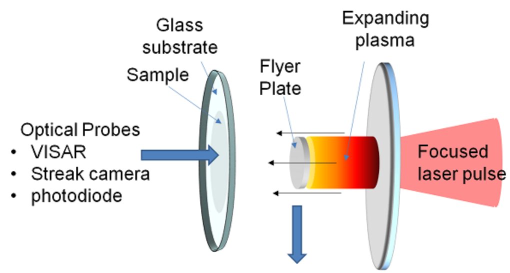


- ***Directly monitor time dynamics of energetic excited state***
- ***Compare with excited states formed from shocks***





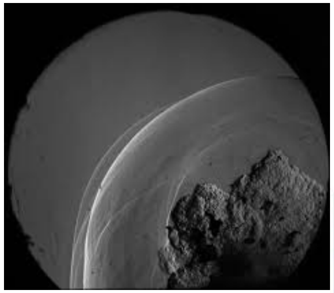
Laser Driven Flyer Plates

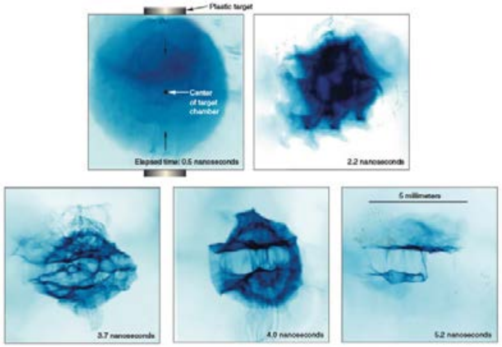


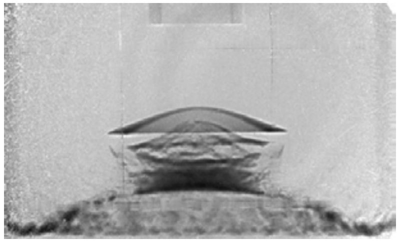
Flyer plate images with 200 mJ laser pulse

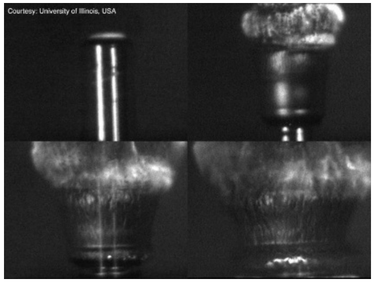
Pushing the limits of explosive characterization

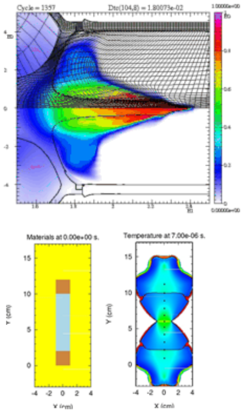
Improved Resolution of events close to reaction time

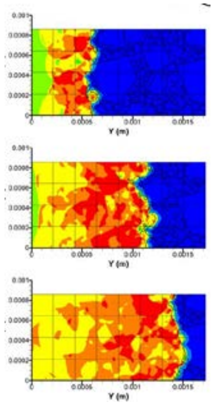




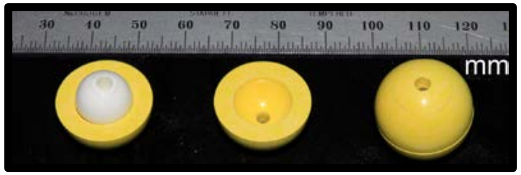


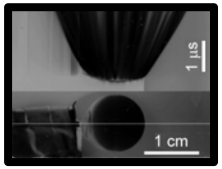


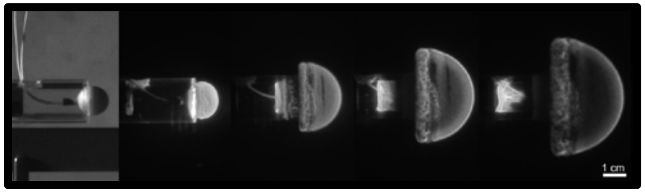


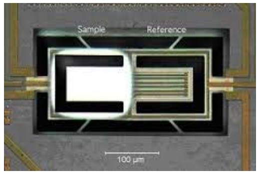


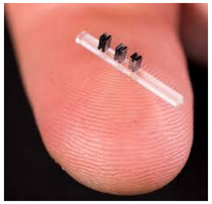
Development of Techniques for Small Scale Performance Characterization



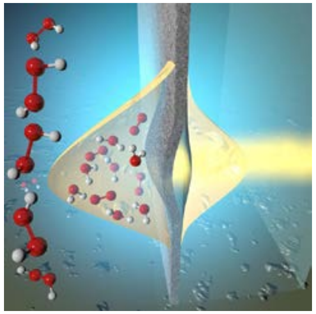








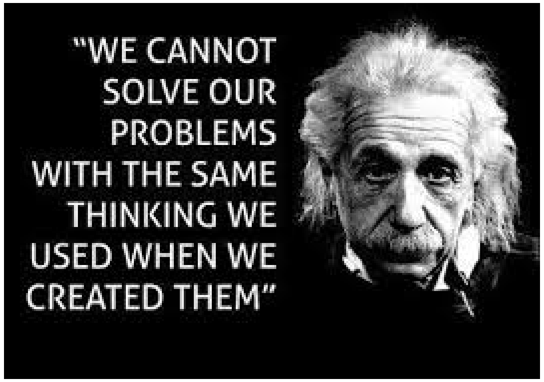
Development of Non-traditional Detonation Tests/Mechanisms



Take Home Messages

- There is enormous, poorly understood, (and fascinating) complexity in the relationship between the fundamental properties and the dependent properties relevant to developing better materials for lethality applications
- Modeling can provide a vector for pursuit but only if the models are continuously improved
- Large area of unexplored capability exists – challenge is low TRL
- Advancing TRL requires a lot of thinking outside the box
- Further development will need long term support but has the potential for BIG payoff

Questions?



Contact Info

Jennifer A. Ciezak-Jenkins

US Army Research Laboratory

RDRL-WML-B

Aberdeen Proving Grounds, MD 21005

410-278-6169

jennifer.a.ciezak-jenkins.civ@mail.mil