



26 August 2008

ARO Chemical Sciences Division



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Dr. Douglas Kiserow

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ARO Chemical Sciences Vision



To identify and enable basic research opportunities in the **chemical sciences** that have the potential to transform Army capabilities and help maintain U.S. technological superiority

To lead the Army by embracing long-term, high-risk, high-payoff opportunities with special emphasis on **Polymer Science, Advanced Energy Conversion, Organic and Inorganic Chemistry, and Physical Chemistry**

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ARO Chemical Sciences



Chemical Sciences Programs

Polymer Science

Advanced Energy Conversion

Organic and Inorganic Chemistry

Physical Chemistry

Program Manager

Dr. Douglas Kiserow

Dr. Robert Mantz

Dr. Jennifer Becker

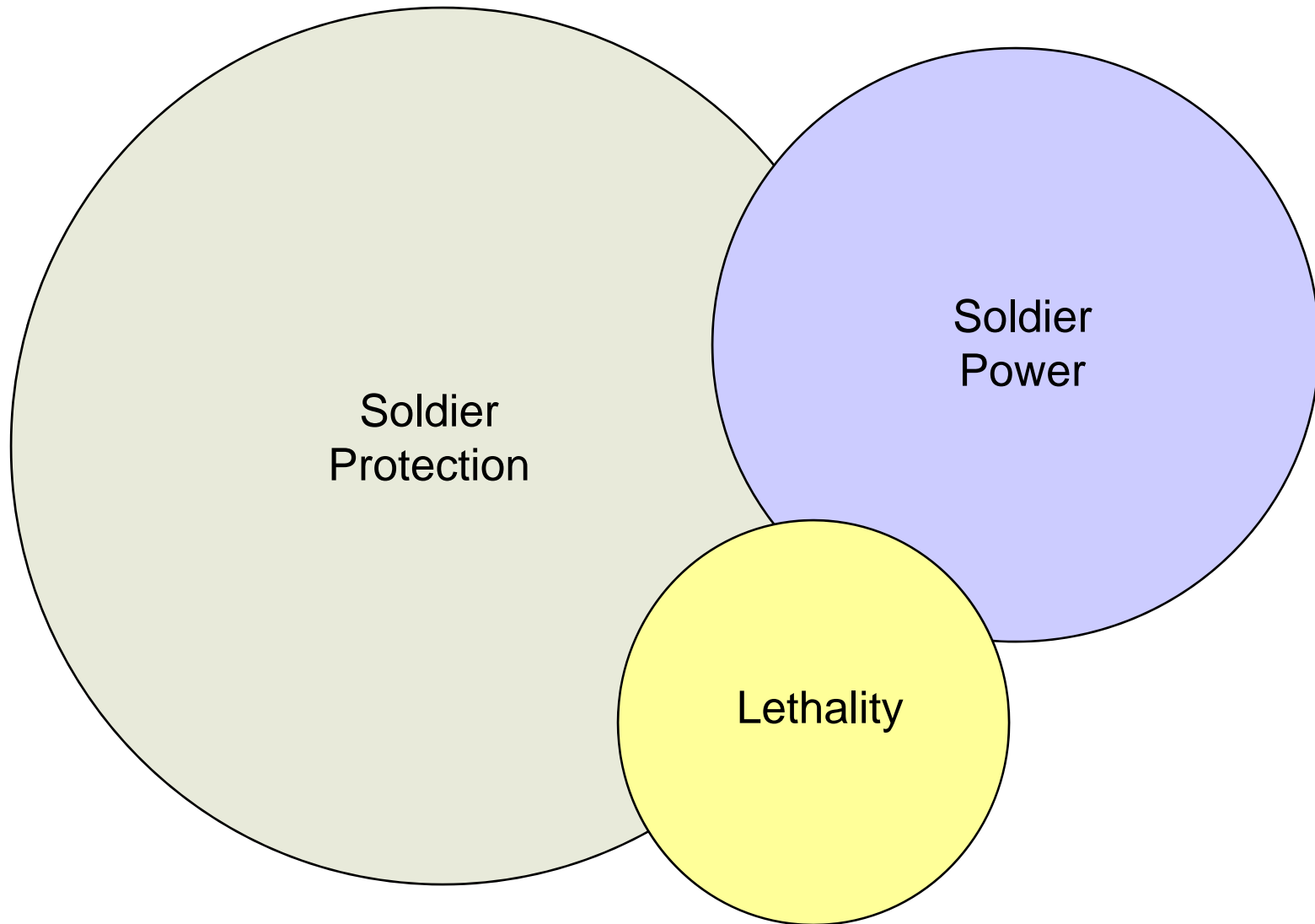
Recruiting

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UNCLASSIFIED ARO Chemical Sciences Army Impacts

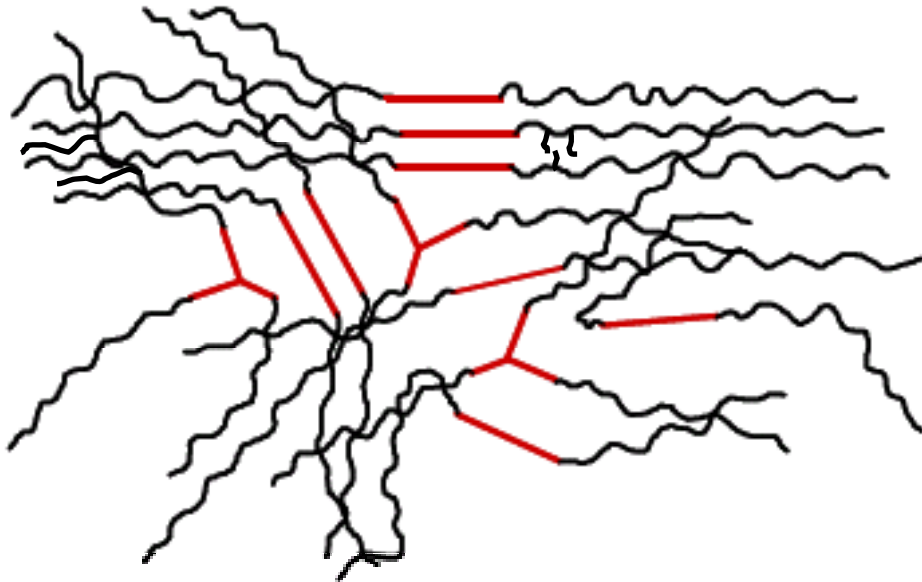


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Polymer Science Vision

To develop a molecular understanding of the complex interplay between macromolecular architecture and functionality such that polymeric materials can be designed to provide the soldier with new and enhanced protection.





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Polymer Science Opportunities



Functionalized Morphology: Control of molecular architecture; precise placement of functional groups in different phases; understand the impact of functional groups across multiple length scales; understand transport in complex systems

New Polymerization Methodologies: Develop new approaches to synthesizing difficult to prepare polymer compositions; develop new reaction conditions for synthesizing polymers

Novel Reactive Monomers: Design and prepare monomers that can generate new polymers with novel properties, including, ionic liquid containing polymers, polymers that exhibit mechanochemical transduction, and selective transport

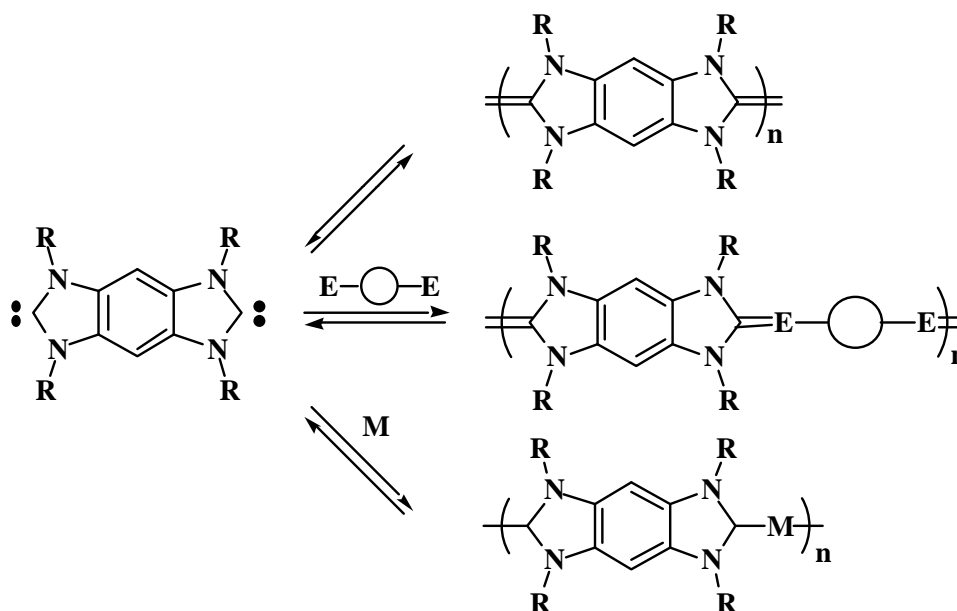
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PI: Christopher Bielawski, University of Texas, Austin

Scientific Goals

- Synthesize new polymers based on N-heterocyclic carbene building blocks
- Design and synthesize dynamic, conjugated polymers that sense failure and undergo self-repair
- Improve conductivity to >1 S/cm (currently 10^{-3})
- Increase healing kinetics



Advanced Energy Conversion Vision

To develop a fundamental understanding of the mechanisms that govern power generation by exploring electrodes, catalysis, electrolytes, and interfaces to provide advanced compact power to the soldier.

The compact power requirements of the future warfighter



Low Power (20 W)

- Communication
- Computation
- Displays
- Weapon sight
- Sensors
- Night vision
- Rangefinder

High Power (100 W)

- Battery charger
- Laser designator
- Microclimate cooling
- Exoskeleton



Advanced Energy Conversion Opportunities



Improved Catalysts: Understand effects of catalysts size, composition, morphology, and support materials on catalyst selectivity and efficacy; identify non-noble metal based catalysts; develop new catalysts that are not poisoned by sulfur.

Advanced Membranes: Understand the transport of species through proton and anionic conductive membranes; develop new polymer and inorganic conductive materials with improved conductivity and chemical stability.

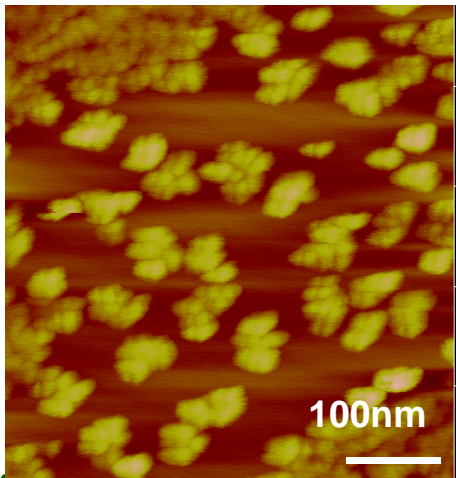
New Reforming Approaches: New methods to efficiently reform hydrocarbons to generate hydrogen.

Novel Battery Chemistries and Materials: New technologies to enable both high power and energy densities for rechargeable batteries.

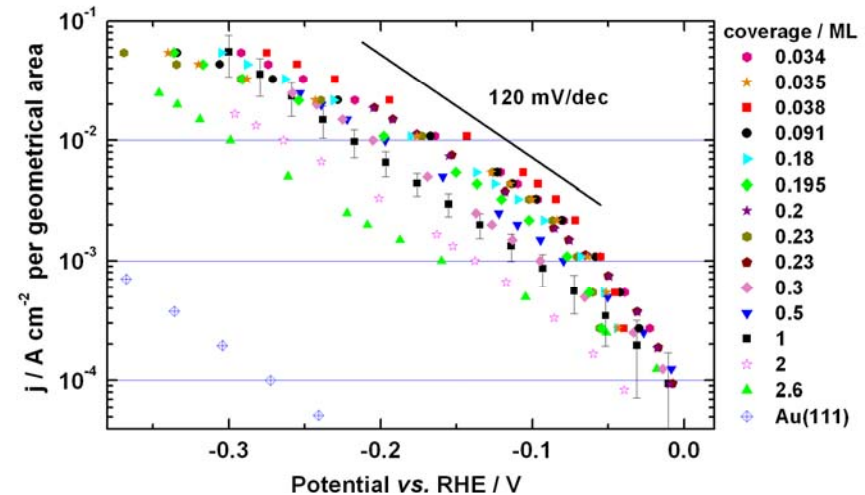
PI: Ulrich Stimming, Technical University of Munich

Scientific Goals

- Understand critical parameters (e.g. particle size, morphology, dispersion) that may influence the activity of fuel cell catalysts
- Understand the influence of the support material
- Reduce the amount of noble metals used in catalysts



**Platinum Islands
on HOPG Surface**

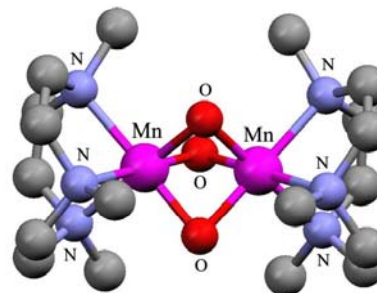
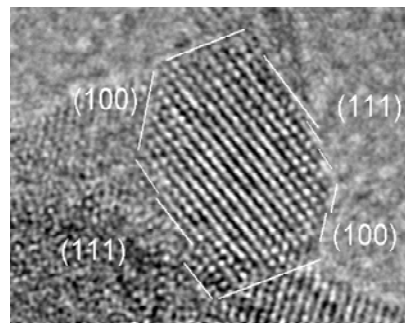


Hydrogen Evolution Reaction Pd/Au(111)

Less Material gives Higher Reactivity!

Organic and Inorganic Chemistry Vision

To develop a molecular level understanding of catalytic reactions, functionalized surfaces, and organized assemblies, leading to new materials and processes to protect the soldier from hazardous materials.





Organic and Inorganic Chemistry Opportunities



Catalysis: Design new catalysts for the oxidation and hydrolysis of toxic chemicals that are active under ambient conditions; understand kinetics and mechanisms of catalytic reactions; design nano-structured catalysts; overcome chemical poisoning; understand mass transport in heterogeneous and immobilized catalyst systems

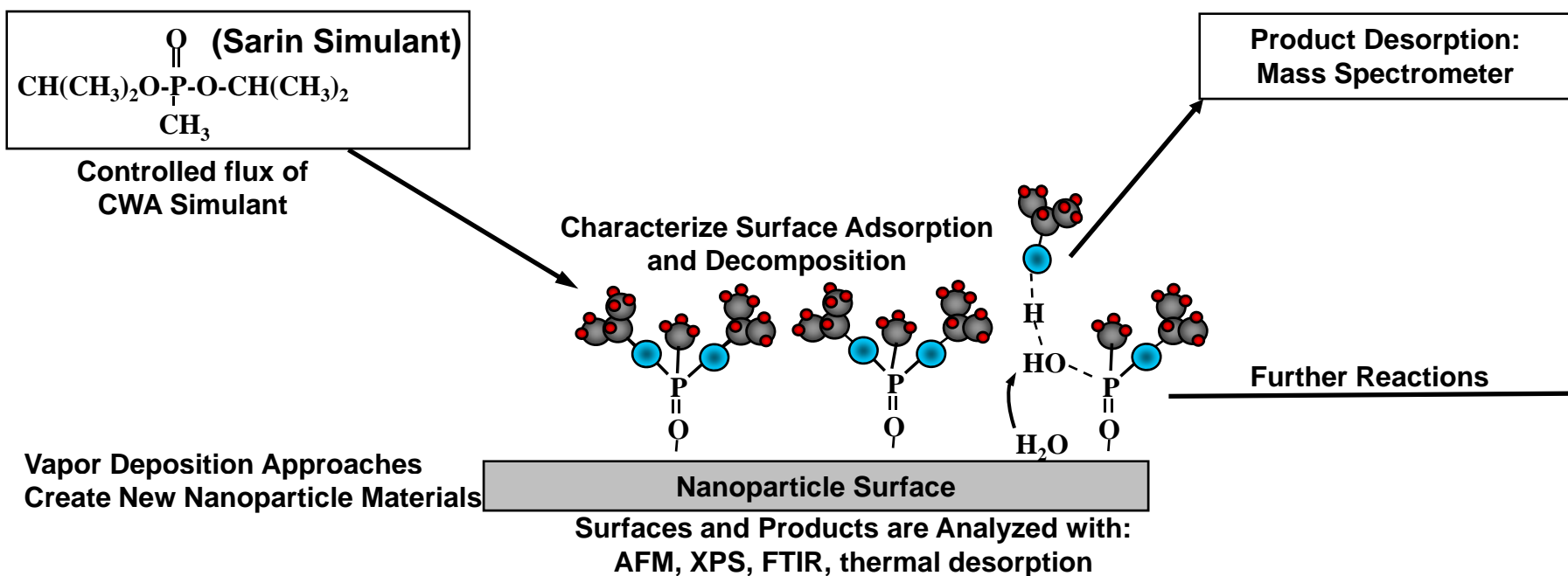
Surface Chemistry: Design and synthesize nano-structured, reactive materials with functionalized surfaces; develop analytical methods for surface and interface characterization; develop mechanistic understanding of chemical fate and mass transport on surfaces

Organized Assemblies: Explore new approaches to synthesize controlled self-assembled structures; control of assembly under various conditions; synthesize functionalized and reactive assemblies; design and synthesize reactive bio-colloids

PI: John Morris, Virginia Tech

Scientific Goals

- Understand how chemical simulants react within single-crystal, nanoparticle, and nanoporous metal oxide materials
- Synthesize high surface area metal oxide nanoparticles
- Determine mechanism of chemical simulant decomposition

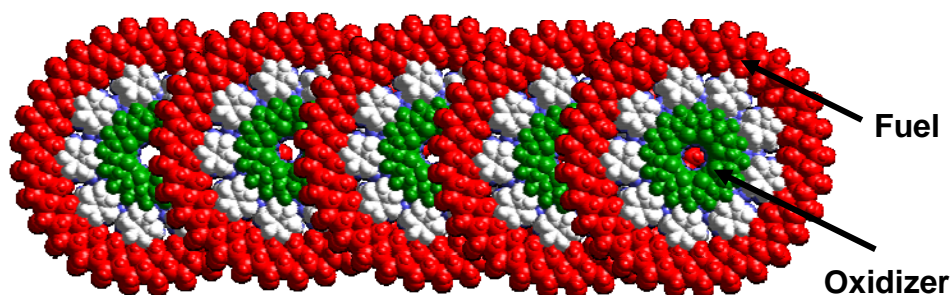


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Physical Chemistry Vision

To advance and exploit recent developments in computational chemistry, molecular and reaction modeling, condensed phase probes, and molecular architecture, leading to new and improved materials for soldier protection and energetic materials.

Nano-engineered energetics



Built from the bottom up for
controlled energy release



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Physical Chemistry Opportunities



Measure and Model Fast Reactions and Materials Properties:

Measure properties early in combustion process at temperature and pressure extremes; develop condensed phase computational chemistry tools; explore new experimental probes

Reactions in Extreme Media: Explore fast reactions in high temperature water; characterize and understand the incineration of military toxic materials

Control of Molecular Motion: Explore molecular control by fast laser pulse shaping; use control for threat detection

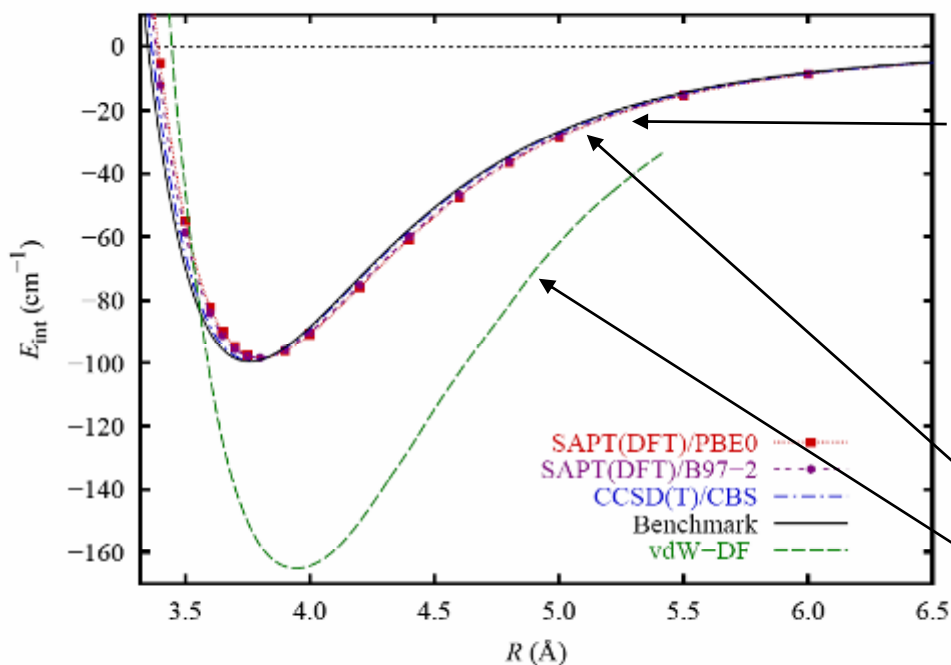
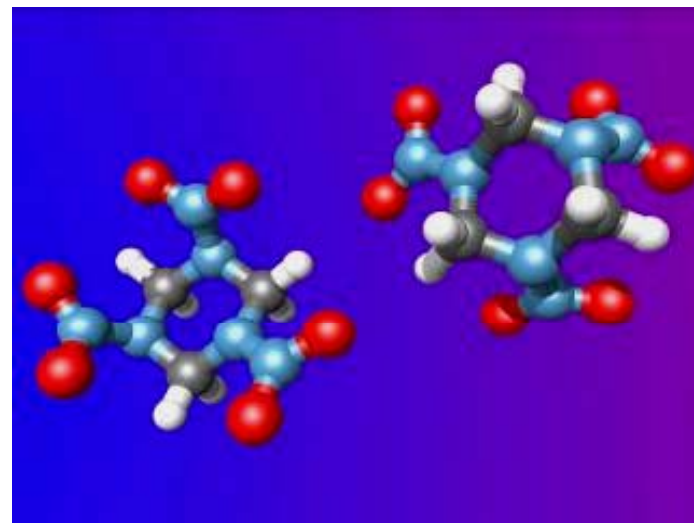
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PI: Krzysztof Szalewicz, University of Delaware

Scientific Goal

To develop a new theory for intermolecular forces, SAPT (Symmetry Adapted Perturbation Theory), to calculate the force between RDX molecules



SAPT has been shown to agree almost exactly with accurate but more complex calculations costing 100X more

CCSD(T) – very accurate, but long computer times and expensive
DF – a common approximation, but poor agreement



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Complimentary RDECOM Chemical Sciences Research



Polymer Chemistry

- ARO Materials Sciences Division
- ARO Mechanical Sciences Division
- ARL-WMRD
- NSRDEC

Organic and Inorganic Chemistry

- ARO Life Sciences Division
- ARO Environmental Sciences Division
- ECBC
- ARL-SEDD
- NSRDEC

Advanced Energy Conversion

- ARO Mechanical Sciences Division
- ARO Materials Sciences Division
- ARL-SEDD
- ARL-VTD
- CERDEC
- NSRDEC

Physical Chemistry

- ARO Mechanical Sciences Division
- ARO Physics Division
- ARL-WMRD
- ARDEC

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