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Cooperative Research Alliance Multiscale Modeling of Electronic Materials (MSME)

Dr. Meredith L. Reed

ARL Opportunities Conference

November 19, 2010

Fairfax, VA



US ARMY

RDECOM



APPROVED FOR PUBLIC RELEASE

Protection

- **Materials and Manufacturing Science for Protection**
- Vehicle Protection
- Individual Warfighter Protection

Lethality

- **Energetic Materials and Propulsion**
- Projectiles, Warheads and Scalable Effects
- **Materials and Manufacturing Science for Lethality**
- Affordable Precision Munitions
- Advanced Weapons Concepts

Human Dimension

- Soldier Sensory-Cognitive Motor Performance
- **Neuroergonomics**
- Social-Cognitive-Cultural Networks
- Human Robotic Interaction
- Human Systems Integration

Survivability/Lethality Analysis

- Ballistic Vulnerability/Lethality
- Electronic Warfare
- Information Assurance and Computer Network Defense
- Systems of Systems

Networks

- Information Sciences
- **Network Sciences**
- Battlefield Environment
- Advanced Computing and **Computational Sciences**



Extramural Basic Research

- Chemistry
- Physics
- Life Sciences
- Network Science
- Environmental Sciences
- Materials Sciences
- Mechanical Sciences
- Mathematics
- Computing Science
- Electronics

Sensors

- RF Technologies
- **Electronics Technologies**
- EO/IR Technologies
- Non-Imaging Technologies
- Sensor Processing

Power and Energy

- Power Generation and Conversion
- Energy Storage
- Power Control and Distribution
- Thermal Management
- **Energy Science**

Mobility and Logistics

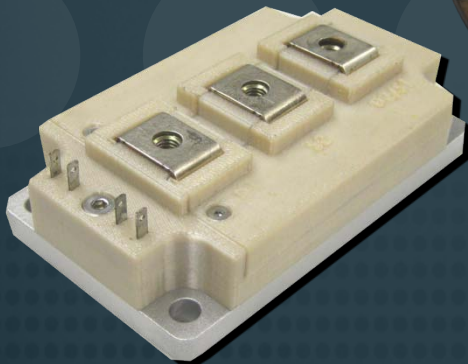
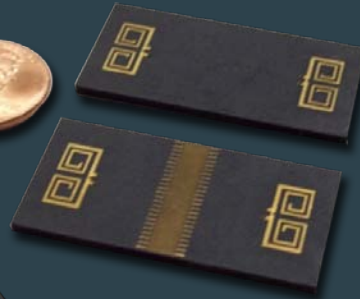
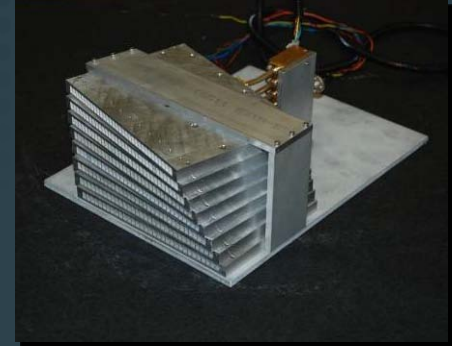
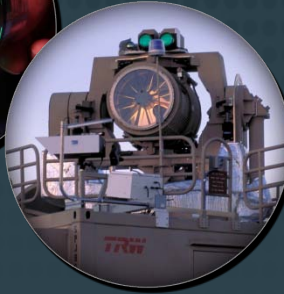
- Platform Mechanics
- Vehicle Propulsion
- **Autonomous Systems**
- Reliability

Simulation & Training

- Intelligent Technologies for Training
- Synthetic Environments
- Immersive Learning
- Training Application Environments
- Advanced Distributed Simulation

Sensors

- RF Technologies
- EO/IR Technologies
- Non-Imaging Technologies
- Electronics Technologies
- Sensor Processing



Power and Energy

- Power Generation & Conversion
- Power Control & Distribution
- Energy Storage
- Thermal Management

ELECTRO-OPTICS & PHOTONICS

**EO Materials &
Devices**

Microphotonics

Optics

**Optics & Photonics
Technology
Integration**

ELECTRONICS & RF

**Micro & Nano Materials
and Devices**

**Electronics
Technology**

**Antennas & RF
Technology
Integration**

**RF Signal
Processing
& Modeling**

SIGNAL & IMAGE PROCESSING

**Acoustics & EM
Sensing**

**ISR Technology
Integration**

Image Processing

**Networked Sensing
& Fusion**

ENERGY & POWER

Electro-chemistry

Power Components

Power Conditioning

**SPECIAL
PROGRAMS
OFFICE**

**SENSORS &
ELECTRONICS
INTEGRATION
TECH OFFICE**



Collaborative Ventures



Network & Info Sciences
International Technology Alliance

Institute for Soldier
Nanotechnologies
MIT

Institute for Collaborative
Biotechnologies
Univ. of California, MIT

Center for Advanced
Microelectronics Manufacturing
Binghamton University

Flexible Display Center
Arizona State University

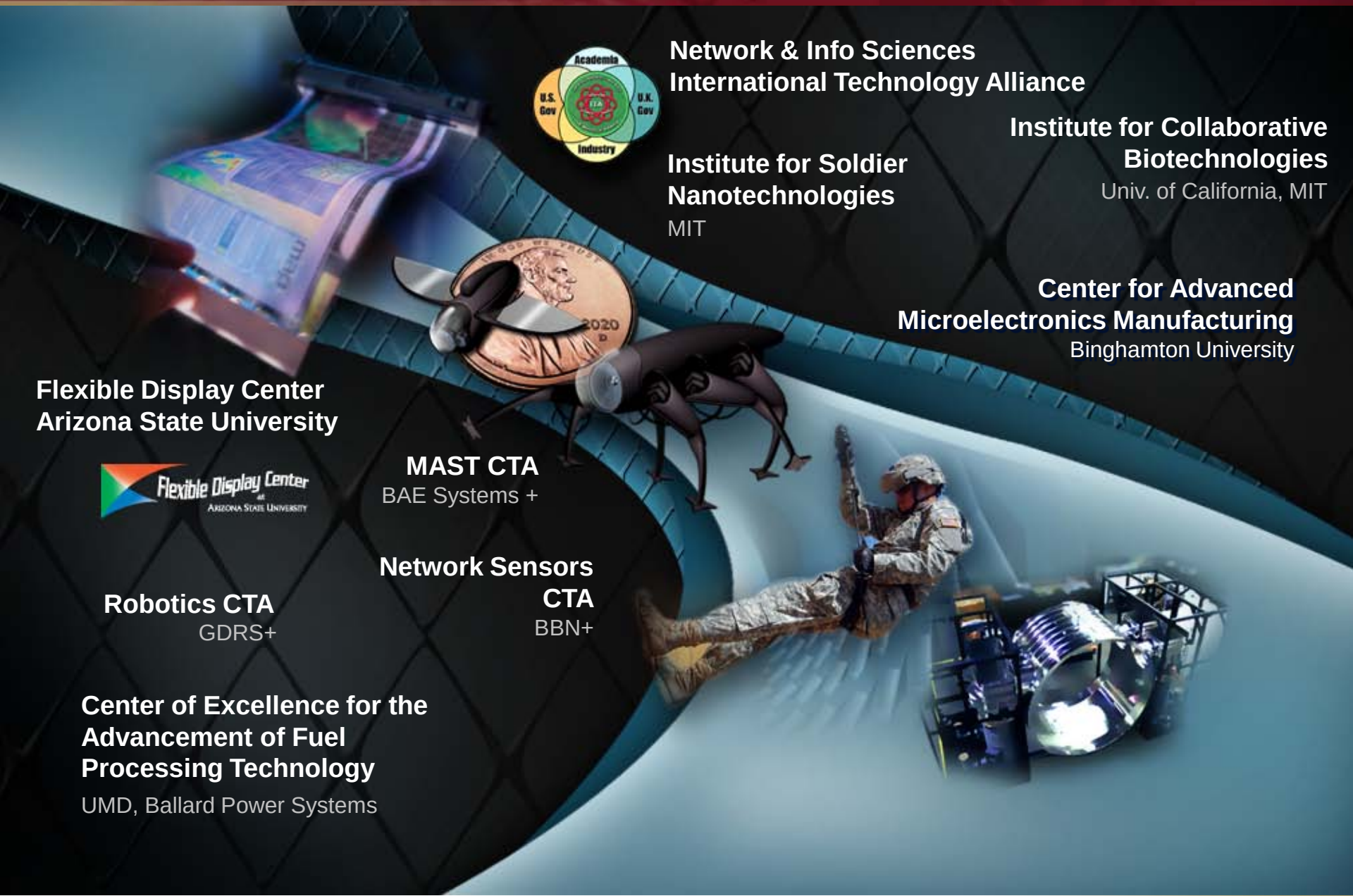


MAST CTA
BAE Systems +

Network Sensors
CTA
BBN+

Robotics CTA
GDRS+

Center of Excellence for the
Advancement of Fuel
Processing Technology
UMD, Ballard Power Systems



Microanalysis

- SEM/EDXS
- Auger/XPS
- SIMS
- AFM
- HR TEM
- FIB
- XRD
- Micro Raman

Bio & Nano

- Bio/Nano Fabrication and characterization (BSL-II)

Specialty Electronic Materials and Sensors Cleanroom

- E-Beam Lithography System
- i-line Lithography
- Lithography Stepper (optical)
- In-Process Material and Device Characterization
- Piece Part to 6" Wafer Capable
- RF Range Facility
- E/B – Field Sensor Suite
- Metal & Dielectric Deposition
- LPCVD High Temperature Processing and Wafer Bonding
- RIE/ICP

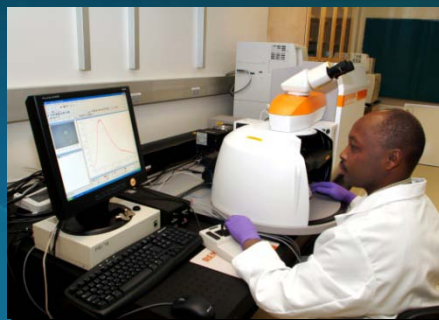
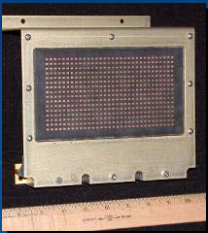
Electro Optics & Photonics

- Time-Resolved Infrared Spectroscopy Facility
- MOCVD, MBE semiconductor growth
 - Indium Phosphide
 - Gallium Nitride
 - Gallium Antimonide
 - Lead Tin Telluride
 - Mercury Cadmium Telluride
 - Gallium Arsenide

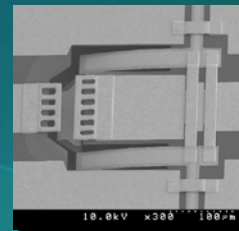
Power & Energy

- Reformer Lab
- Power Conditioning Lab
- Energy Storage Labs
- Micro Power Lab
- Power MEMS

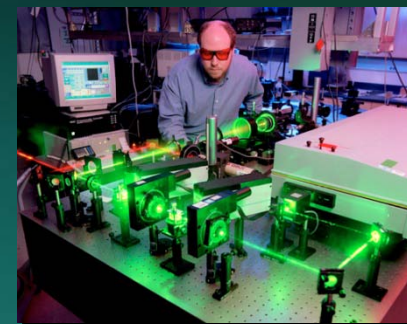
Radar, Antenna & MFRF



**Spectral
dissection of
bacteria and
thin-films**



**NEMS &
MEMS PZT**



Non-linear Optics



**RF Material &
Devices**



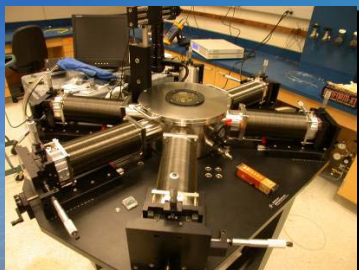
**Electric
Field Cage
for sensor
evaluation**



**Piezoelectric
Sputtering for
MEMS and
communication
devices**



**Device Fabrication
Advanced RF
Technology**



**DC-40GHz
environmental
cryogenic I/V
probe station**

**Electronic
transport
characterization in
nano-scale
structures**



**III-V Etching
for optical
device
fabrication**



**Device
Fabrication
Electro-
Optics**





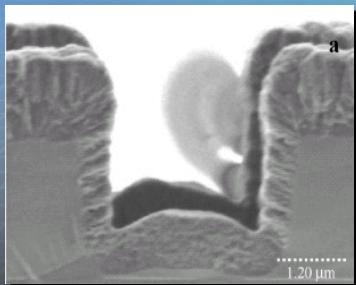
Jet Vapor Deposition



**Dry Room for
electrochemical
cell preparation**



**Power Conditioning
Lab**



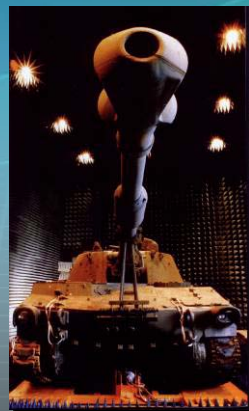
**SiC device stress
analysis evaluations**



**Air Gun for high-G
evaluation**



**Isomer Battery
Laboratory**



**High Power RF
Anechoic
Chamber**



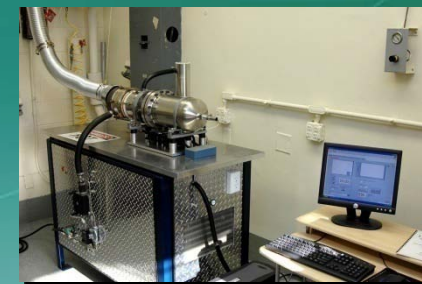
**Single and
multiple
battery cell
evaluation
laboratories**



**Fuel Cell
evaluations**



Electric Drive



**Small Engine
Evaluation**



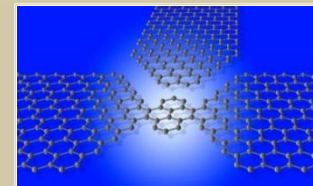
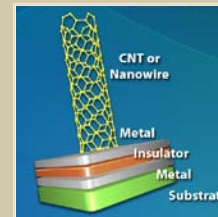
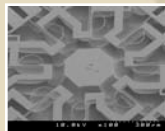
**Fuel Cell
Powered
Robotic Vehicle**



Area
Surveillance
and Tracking



MEMS
Sensors and
actuators for
microrobots



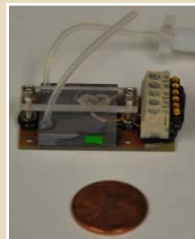
Graphene



**Family of
UGS**



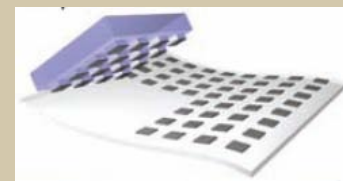
Compact Radar



**Wide
Bandgap
Devices**

**Environmental
Sensing**

**Energy Harvesting
Rectenna**



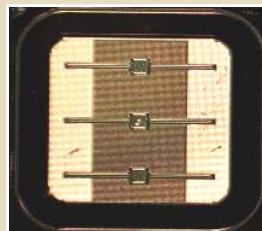
Flexible Electronics



**Reformed
Methanol
Fuel Cell**



**Traction Module
Power Conversion
Switches**

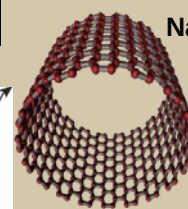


**Li-Air Prototype
Cells**

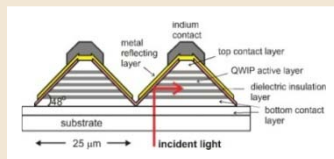
**Isotope
Energy
Source in a
AA-battery
Package**



**Carbon
Nanotubes**

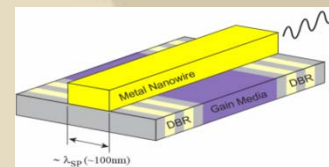


**C-QWIP
FPAs**



**Flexible
Displays**

**High Voltage
Li-Ion
Electrolytes**



**Photonics &
Electronics Integration**

Accomplishments

Near Term

Future

**Disruptive Sensors and Electronics for C4ISR Superiority and
Advanced Energy and Power for Warfighter Dominance**

STRATEGIC DIRECTION

(Networks, Signal Processing,
Social, Environmental, Battle Plan, etc.)

Data to Decisions

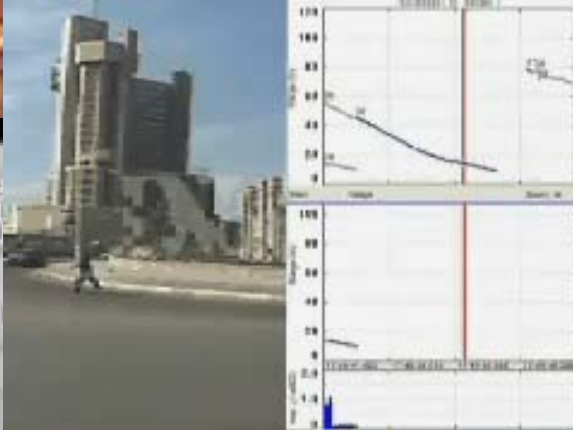
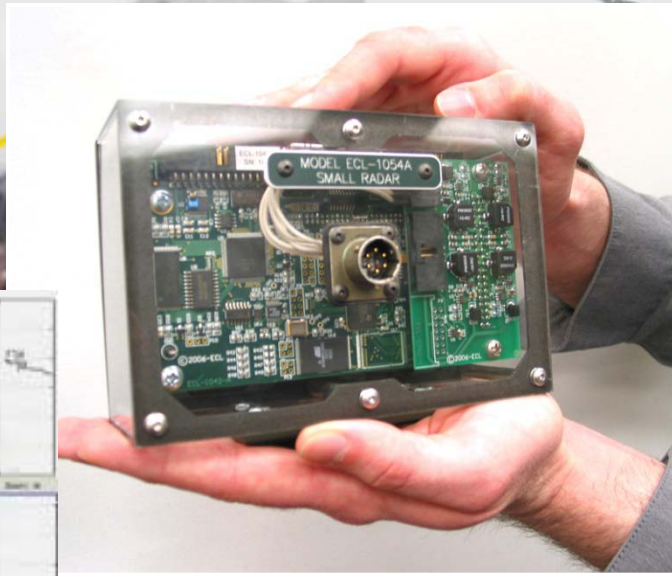
Persistent Surveillance

Unique Electronics for Battlespace
Effects, Sensing and Processing

Ubiquitous Efficient Energy

Warfighter Outcomes

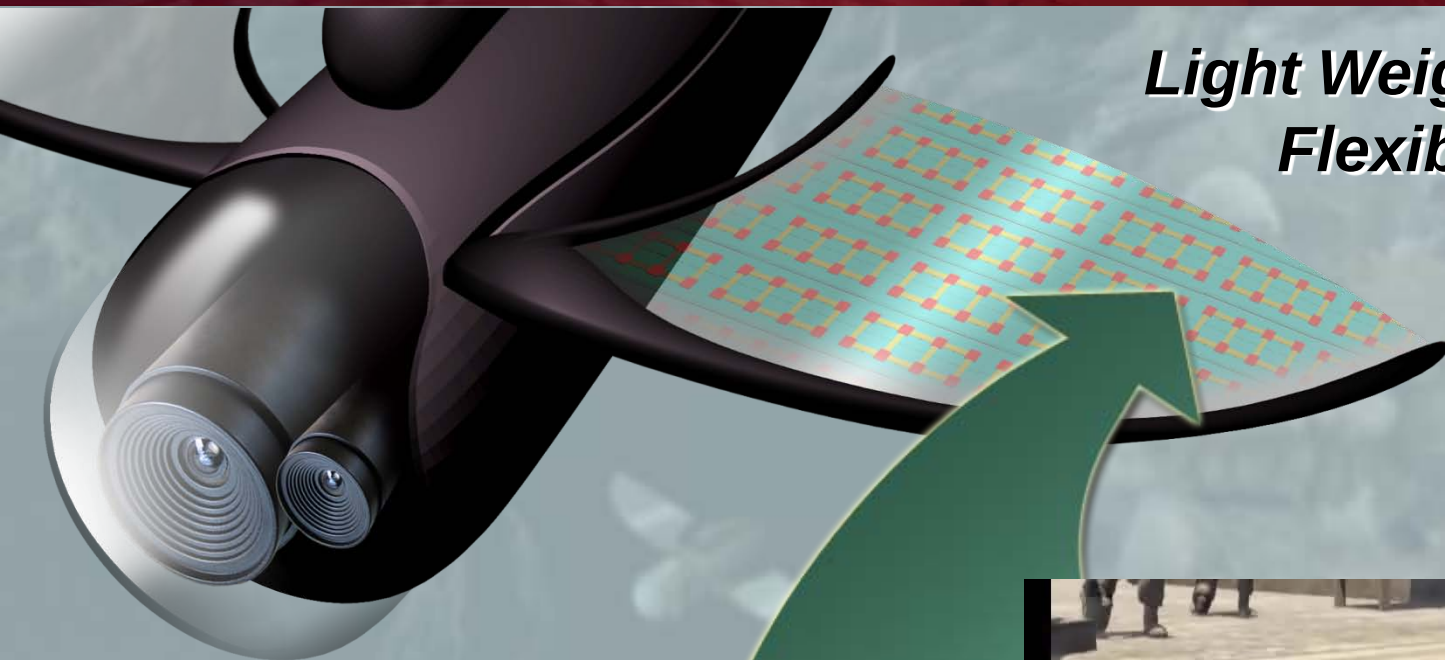
- Counter IED & Mine
- Mission Command
- Training
- Power & Energy
- Human Dimension
- Force Protection
- Battlespace Awareness
- Force Application
- Logistics
- Unmanned Systems Operations



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*Light Weight,
Flexible Electronics*



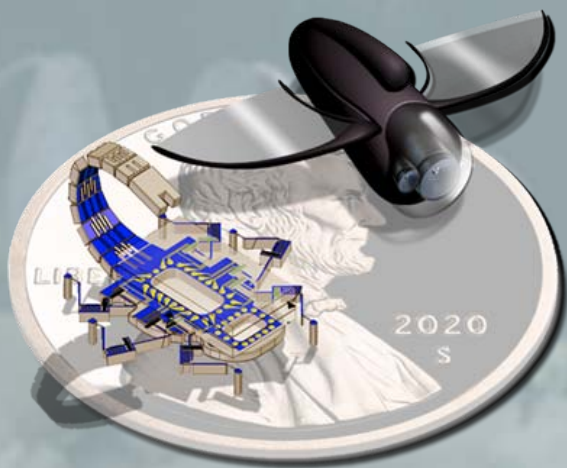
CMOS, Pro
Logic, D

Source



Gate Electrode

Flexible Substrate





Multi-Scale Mat. Behavior in Ultra High Loading Rate Environments

- Investigate bridging scales
- Develop models & simulations
- Develop innovative experimentation & validation techniques
- Define multiscale material metrics
- Perform processing & synthesis

Electronic Materials

- Explore material designs for electrochemical energy,
- Develop hybrid photonic, spintronic devices
- Investigate and develop heterogeneous metamorphic electronics

Protection Materials



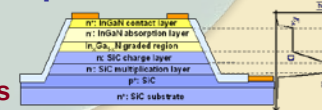
**Designer
Microstructure
Composites**

Army-relevance

Underpinning
science infusion

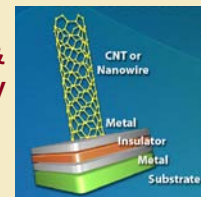
Army-relevance

Electronics



Opto- electronics

Power & Energy



In-house Cross-Disciplinary Multiscale Research of Materials Initiative

- Underpinning Multiscale Physics & Chemistry Fundamentals
- Computational Science Environments, Codes & Software Tools
- Validation & Verification

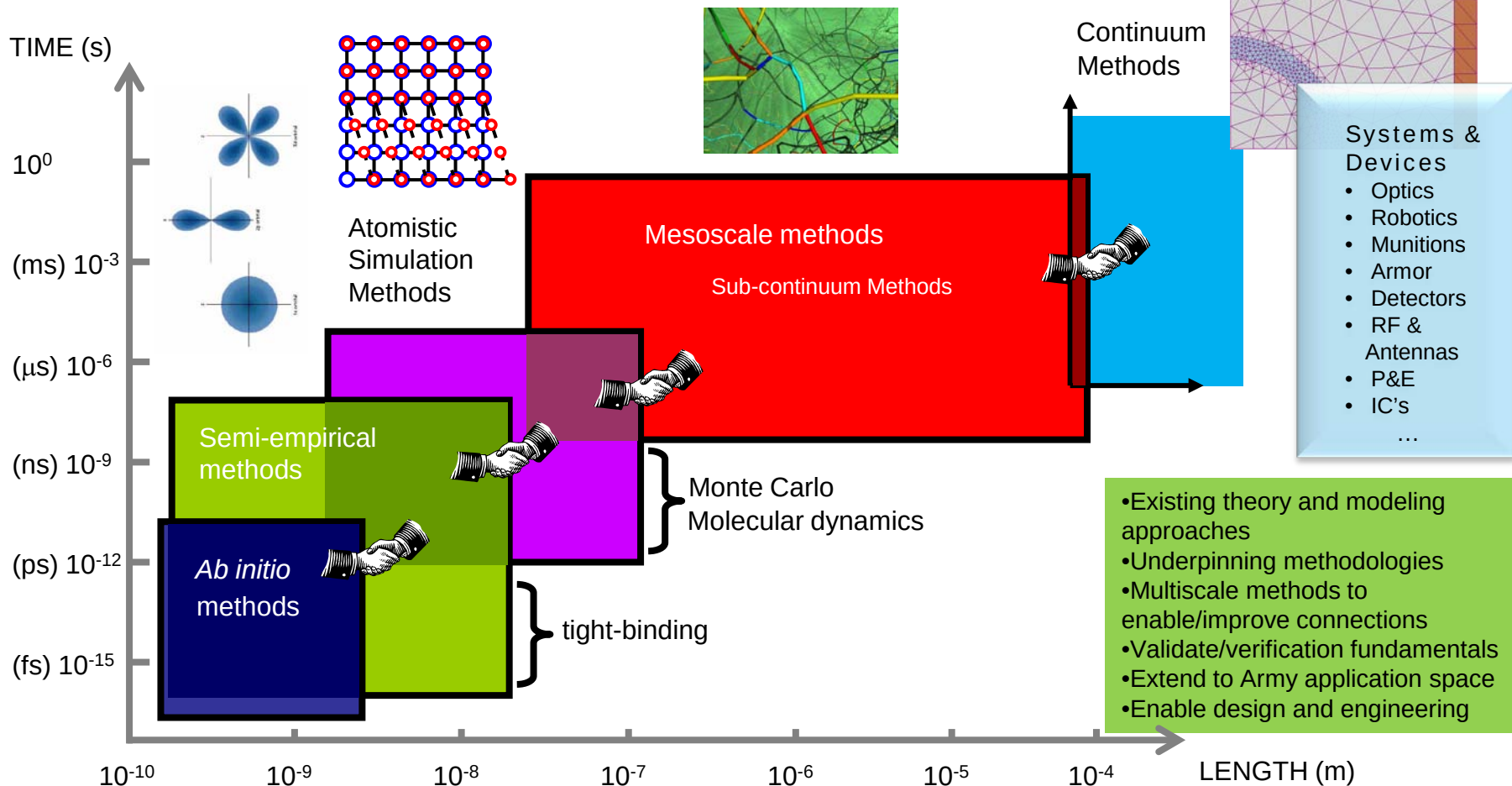


Motivation

Multiscale Modeling of Electronic Materials

- To enable the quantitative understanding of electronic materials from the smallest to the largest relevant scales
- Resulting models are needed to create new understanding and improved electronic device applications to include sensors and electronics for enhanced battlespace effects, and efficient power and energy devices

Challenge: modeling physical phenomena from a broad range of perspectives, from the atomistic to the macroscopic end (and **back**)



Large jumps are easier than smaller intimate jumps.

LIGHTER FOCUSED.

ARL Multi-Scale Multi-Disciplinary Modeling of Electronic Materials Workshop

Aug 31 – Sep 1 2010

Fairfax, Virginia 22033

Opportunities for Multiscale Modeling of Electronic Materials

Electrochemistry

Focus on interfacial physics and chemistry; nano structures, solid-liquid interface—clear opportunities for batteries, capacitors, fuel cells, etc.

Photonic Interactions

Interaction of photons, electrons, phonons—in other words, photonics, spintronics, plasmonics, and phonons

Heterogeneous Metamorphic Electronics

Mixed materials, with partial ordering—includes graphene, metamaterials, nanoelectronic structures, etc.

Objectives

- **Execute a focused basic research program to realize a materials by design capability**
- **Drive forward and expand the fundamental understanding in the area of multi-scale/multidisciplinary materials behavior to directly improve the performance of electronic materials.**
- **Create a framework that enhances and fosters cross disciplinary and cross organizational collaboration that brings a team of academia, industry and government together to address critical focused research in Multiscale Modeling of Electronic Materials**



Electrochemistry

Focus on interfacial physics and chemistry; nano structures, solid-liquid interface—clear opportunities for batteries, capacitors, fuel cells, etc.

Photonic Interactions

Interaction of photons, electrons, phonons—in other words, photonics, spintronics, plasmonics, and phonons

Heterogeneous Metamorphic Electronics

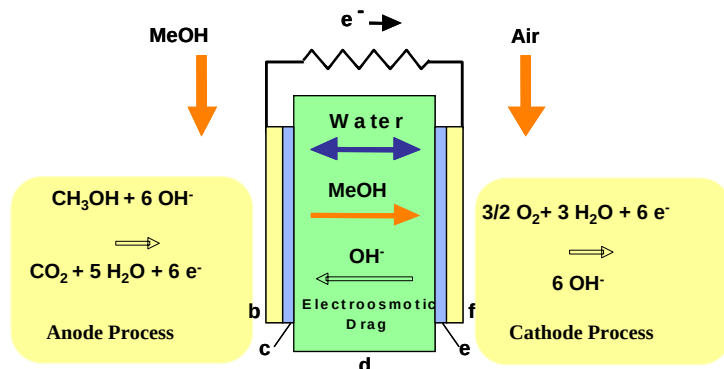
Mixed materials, with partial ordering—includes graphene, metamaterials, nanoelectronic structures, etc.

- Interfaces of dissimilar materials
- Defects

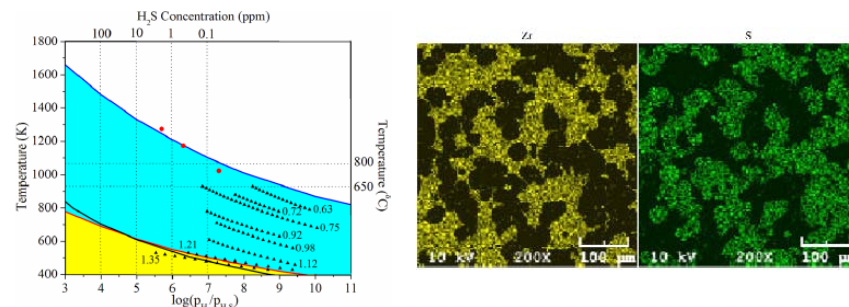
Note: Asking for CRA proposals to include a plan for incorporating “Hybrid Organic Electronics” in future years



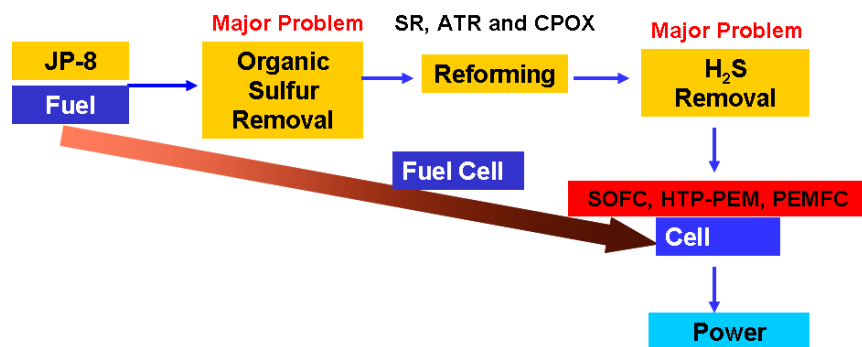
Alkaline Membrane Fuel Cells



Long-Term Interest – Solid Oxide Fuel Cells

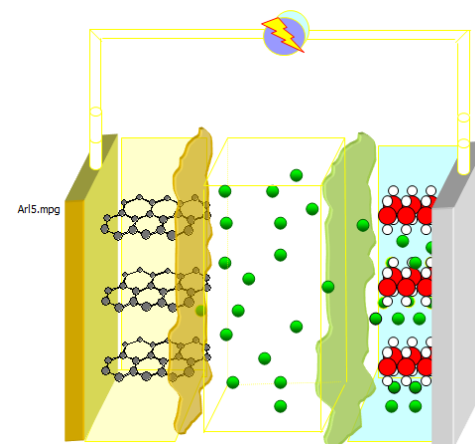


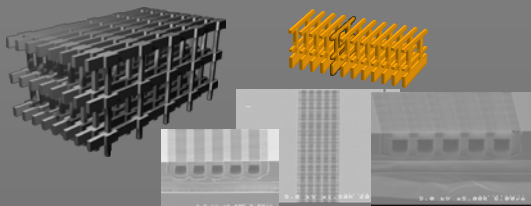
Logistics Fuel Processing



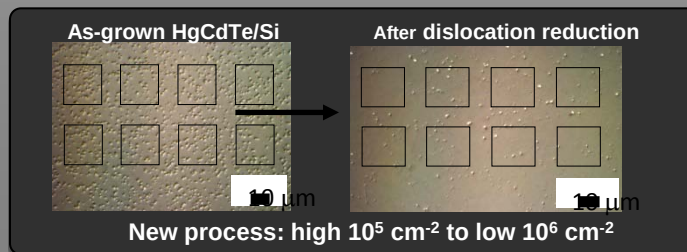
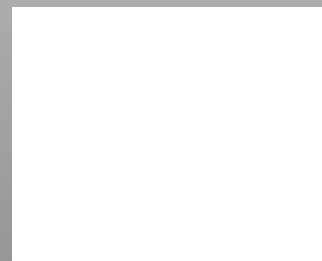
Li-ion Batteries

- Energy density: 200 Wh/kg; Power density: 4 kW/kg at 60 Wh/kg
- Insertion types of cathode and anode for high rechargeability
- Protective solid electrolyte interphase (SEI) for long cycle and storage life

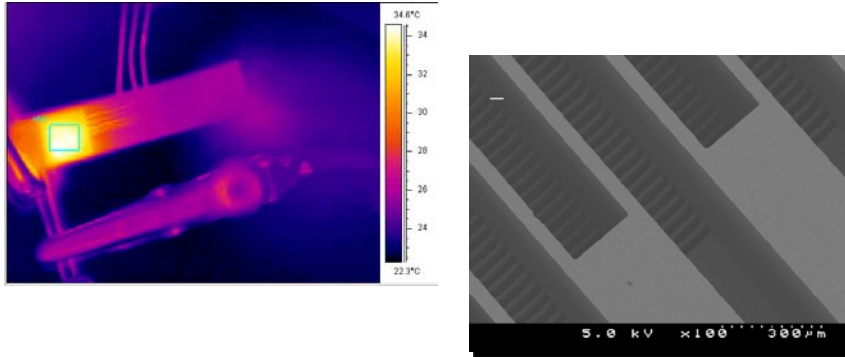




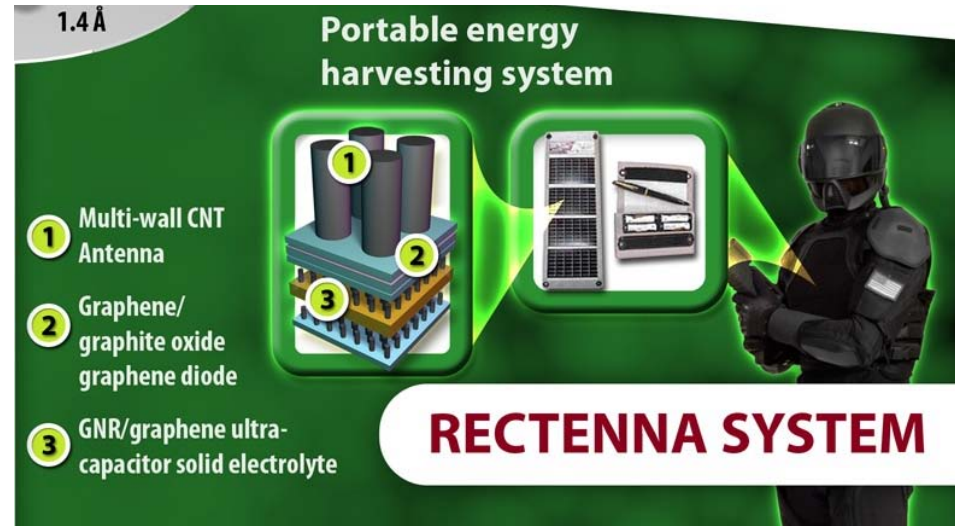
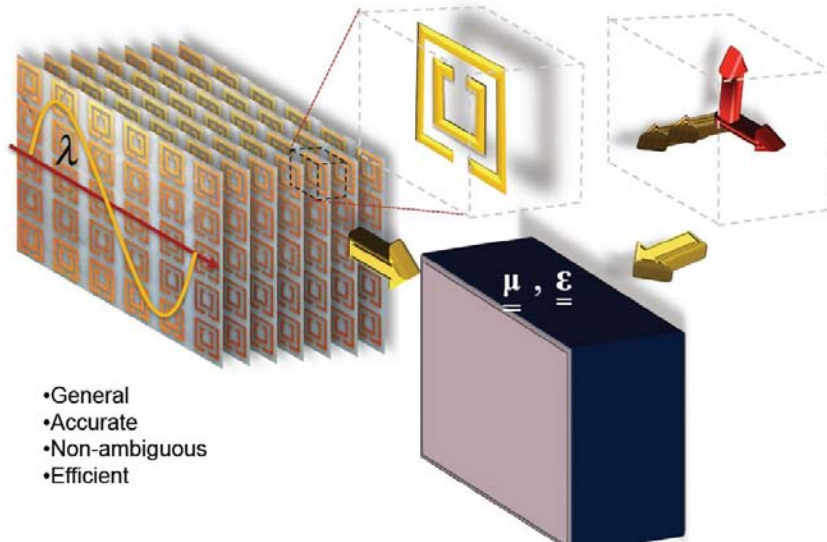
III-Nitrides



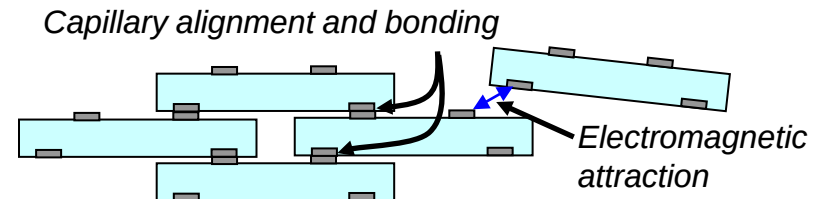
WBG Semiconductor Power Devices



Meta-materials for RF/Antennas

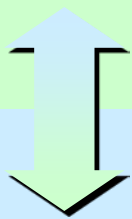


Heterogeneous Integration via Fluidic self-assembly



Multiscale Modeling Research Areas: Performed for each of the Electronic Materials Research Areas

External
CRA
Effort



ARL
CRA
Effort

- **Modeling and Simulation:** Validated multiscale modeling of electronic materials design materials and predict performance by exploiting the hierarchy of scales in a multidisciplinary environment
- **Bridging the Scales: Analysis, Theory and Algorithms:** Validated theoretical and analytical analyses to effectively define the interface physics across length scales and disciplines
- **Multiscale Modeling Material Metrics:** A comprehensive set of metrics that electronic material for each of the three Electronic Materials Research Areas defined above to enable the enhancement or creation of new electronic devices
- **Validation and Verification:** Comprehensive validated experimental capabilities bridging time and space for probing the physics and mechanisms of electronic materials and for verification and validation of multiscale/multidisciplinary physics modeling.
- **Processing and Synthesis:** Validated modeling and techniques for the synthesis and processing of Electronic Materials.

Approach

Cohesive, multidisciplinary collaborative research program that links Electronic Materials across length & time scales to specific performance metrics by validated modeling, characterization and processing

Electronic Materials for U.S. Army Systems

Multiscale/Multidisciplinary Materials Design Loop

Modeling & Simulation (1)

Verification, Validation and Prediction across multiple scales

Bridging the Scales (2)

Theoretical and analytical analysis to define the interface physics across scales

Electronics and Sensors for Enhanced Battlespace Effects and Efficient Energy & Power Devices

Processing and Synthesis (5)

Novel techniques to achieve new and improved electronic materials

Validation and Verification (4)

Experimentation and Characterization of Electronic Materials for verification and validation of multiscale physics modeling

Multiscale Material Metrics (3)

New and novel metrics to define characteristics and properties



MSME CRA Program Announcement (PA)



- Formulate a program to demonstrate the ability to achieve the research and programmatic goals of the CRA as outlined in the PA
- Define and outline the strategy for executing the materials by design loop and identify how the program will achieve the specific research goals in the five Multiscale Modeling Research Areas and how they will be integrated and interfaced within the materials by design loop
- Identify how the program will address the five Multiscale Modeling in each of the three Electronic Materials Research Areas: (1) Electrochemical Energy Devices; (2) Hybrid Photonic, Spintronic Devices; and (3) Heterogeneous Metamorphic Electronics
- Define the metrics by which success is expected to be measured
- Identify the strategy, plans and methods for collaboration essential to the success of the CRA
- Identify the optimal scientific, technical, programmatic and administrative team (expected to be comprised by a number of members) with the expertise to achieve the stated research goals and to oversee and manage finances, reporting, data, meetings, reviews and intellectual property

Collaboration to Achieve the CRA Research Goals

- **ARL Enterprise for Multiscale Research of Materials**
- **ARL SEDD Mission Program Internal to the CRA**

Education

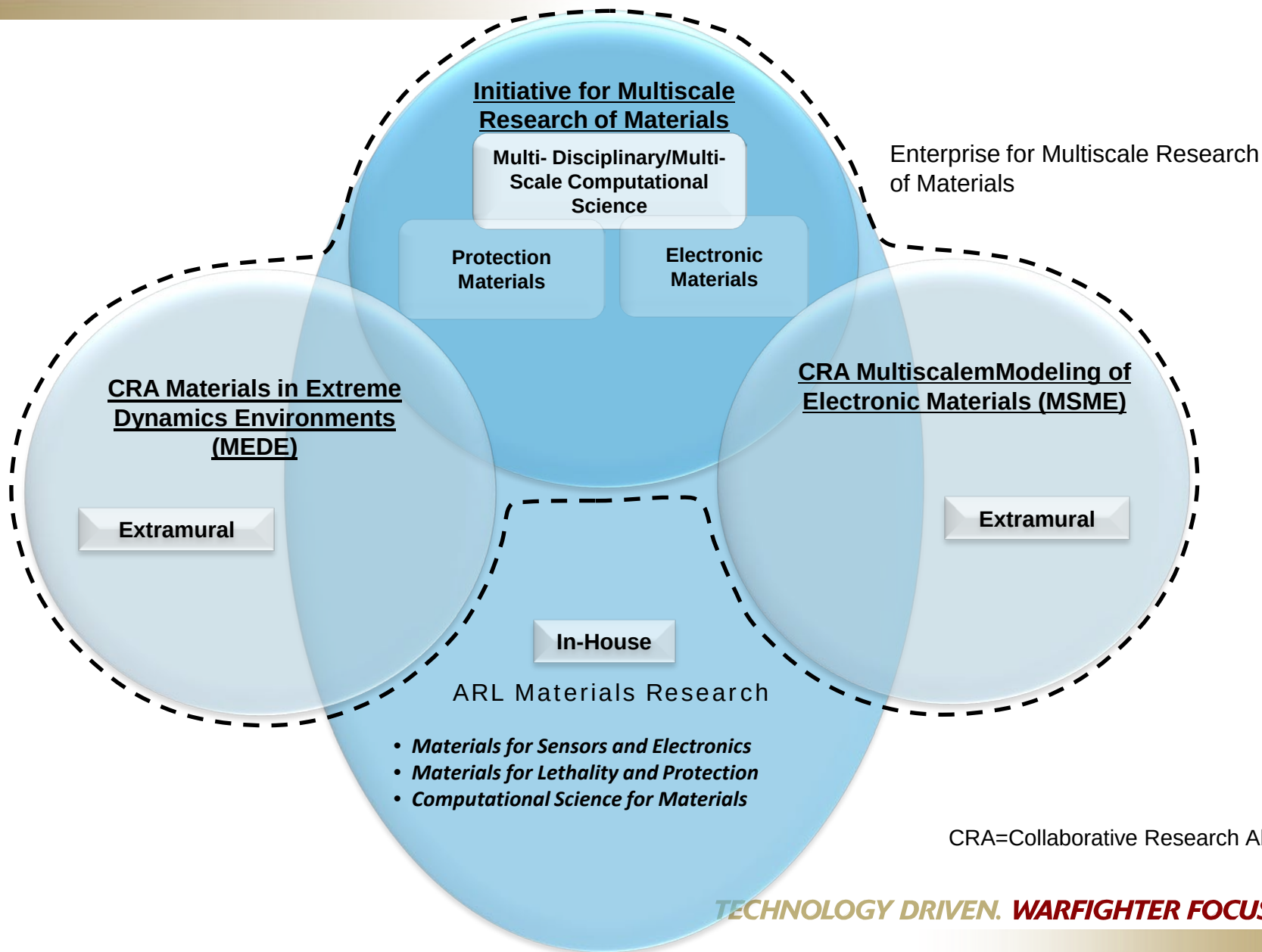
- **Opportunities for Government Personnel**
- **Student Engagement with ARL Research Environment**

Other Collaboration Opportunities

- **High Performance Computing DoD Supercomputing Resource Center (HPC-DSRC)**
- **HPC (High Performance Computing) Software and Application Institute (HSAI) for Multi-Scale Reactive Modeling and Simulation of Insensitive Munitions (MSRMS-IM)**
- **Other Government Agencies (OGA's)**

Lectures, Workshops, and Research Reviews

Staff Rotation



CRA Basic Research Program

- Basic Program funded for 5 Years with a 5 Year Option
- Start Second Quarter FY12
- Budget includes research costs, costs to manage the program, costs to collaborate and enable research transition
- Funding outlined in the PA are for planning purposes only
- Final funding is subject to Program Objective Memorandum Approval

CRA Enhanced Basic and Applied Research Program

- As the CRA proceeds it is anticipated that other Government agencies will be able to provide funding for specific research of interest
- This is currently unfunded

Total Funded 5 Year Core Program \$12.4M /Total Funded 10 Year Core Program \$20.9M



SEDD MSME Open House

Thursday December 9th 2010

8:30 - 9:00 Arrival

9:00 - 12:00 SEDD Research Program and Tours

**Army Research Laboratory-Adelphi Laboratory
Center**

**2800 Powder Mill Rd
Adelphi, MD 20783**

Create a framework that enhances and fosters cross disciplinary and cross organizational collaboration that brings a team of academia, industry and government together to address critical focused research in Multiscale Modeling of Electronic Materials

2 Year Goals

- Advance the fundamental understanding and implementation of Physics-Based Modeling of Electronic Materials across both time and space to develop set of algorithms/theories for a broad range of electronic materials to create new and/or improved electronic devices, and advance the understanding of existing performance
- Introduce interfaces, defects, imperfections

5 Year Goals

- Integrate new multidisciplinary /multi-scale physics to enable multi-scale modeling and simulation capability that is validated experimentally in time and space to apriori design new or improved electronic materials that are uniquely characterized, synthesized and processed.
- Potential examples of enhanced SoA resulting from the advancement or development of new theories and algorithms of MSME could include:
 - Higher performing (longer-lived) batteries by ~ 30% with more than double to treble the energy density
 - Increase efficiency by 20%, with a five fold increase in lifetime for UV solid state sources

10 Year Goals

- Advance the state of the art in multiscale modeling and electronic materials to create a capability for "Materials Optimization and Materials by Design"
- Deploy Multiscale Models for a variety of electronic materials that can be shared within the scientific community