

Multifunctional Carbon Nanomaterials

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“Multifunctional”

- What is “multifunctional”?
- What does multifunctionality have to do with nanomaterials?



- What are the advantages of multifunctional design?
 - Weight Savings
 - Space Savings
 - Redundant Cost Savings

Approaches to Multifunctionality

Combined Functionality



FedEx



Kinko's



FedEx Kinko's
Office and Print Center

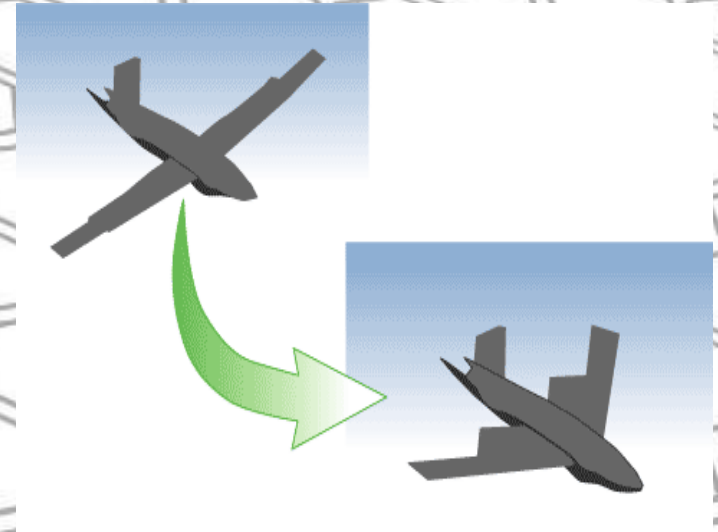
- Remove redundant components
- Reduce size/weight/cost of functional components
⇒ cram more functions into the same unit



Approaches to Multifunctionality

Adaptive Reconfiguration

- Changes properties dynamically
- Performs each function as needed (not all at once)

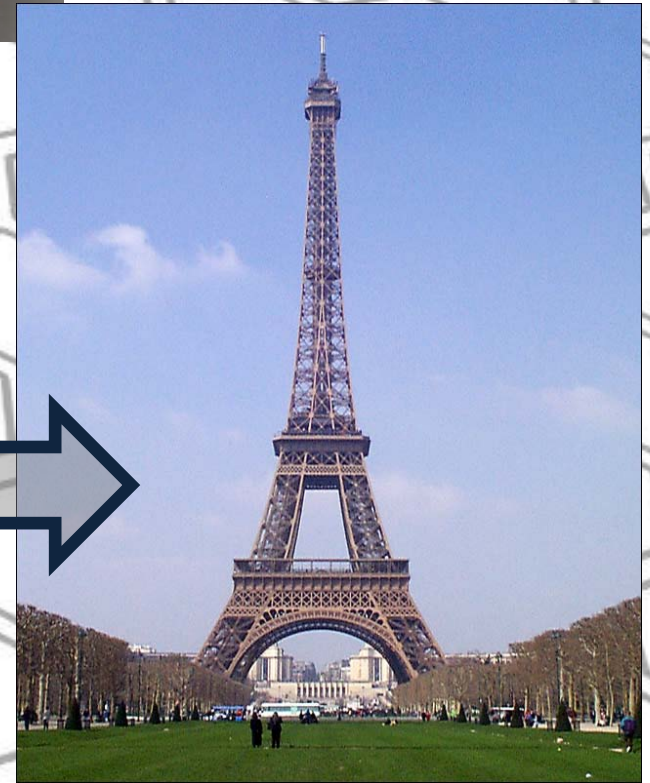
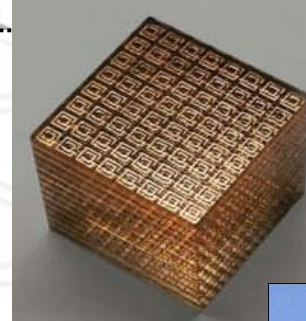


- Shape Change
- Conductivity Change
- Mechanical Properties Change

Approaches to Multifunctionality

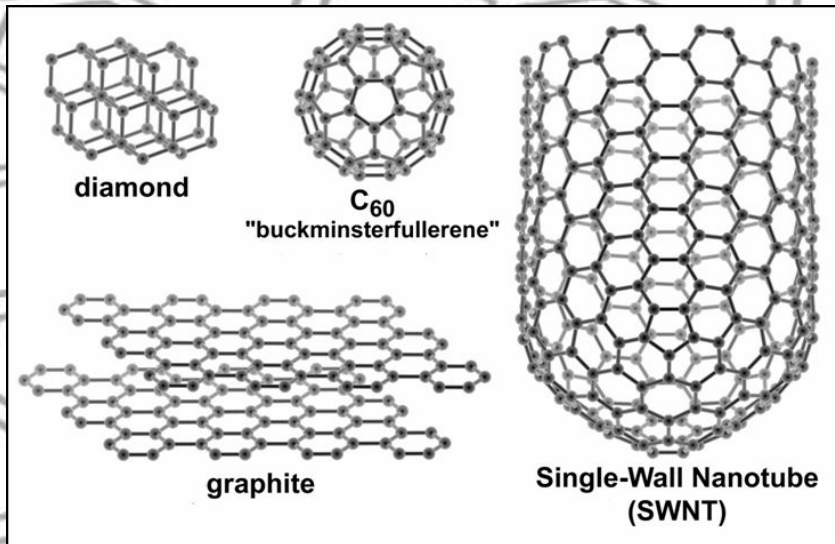
“Metamaterials”: Architecture Driven Properties

- Materials properties driven by geometric construction rather than bulk aggregation
- Manipulate the topology of the relevant fields within the architecture
 - Optics – Electrodynamical Fields
 - Mechanical – Stress/Strain Fields

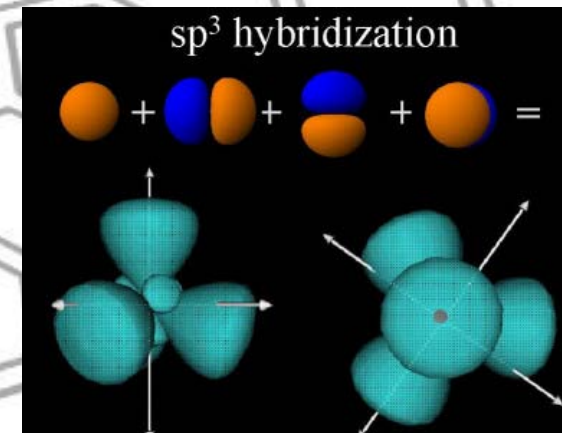
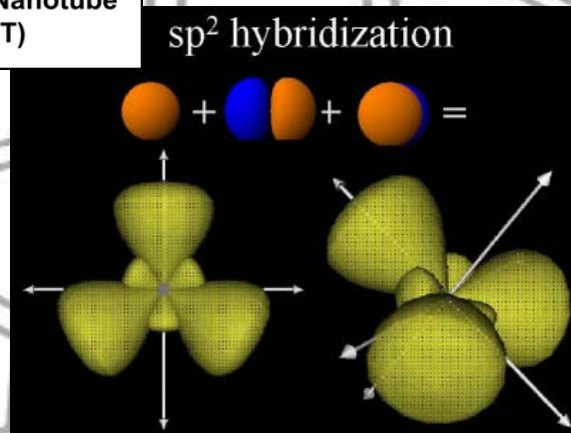


Carbon Nanomaterials

The Carbon Bond



- Diversity
 - sp , sp^2 , sp^3
 - Delocalized π -bonding
- Size/Energy/Delocalization
- Electronegativity & covalence



Multifunctionality from Carbon Nanomaterials

Carbon Properties

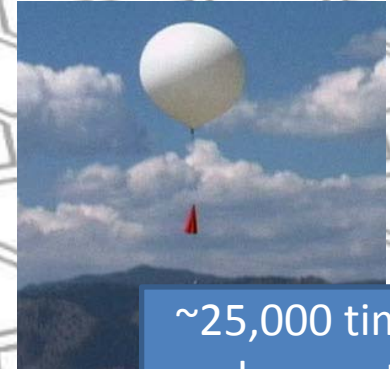
~Diamondoid/alkane : Graphene/Alkene:
Alkyne

- Mechanical
- Thermal
- Electrical
- Chemical
- Nano/Microstructure Modification
 - Polymers (e.g. polyurethane)
 - Ceramics
 - Metals (e.g. aluminum)

- High performance density⇒
Function miniaturization
- Diverse functionality from
diverse allotrope structures
- Matrix phase structure
modification

Nanocomposites: “Percent Contributions”

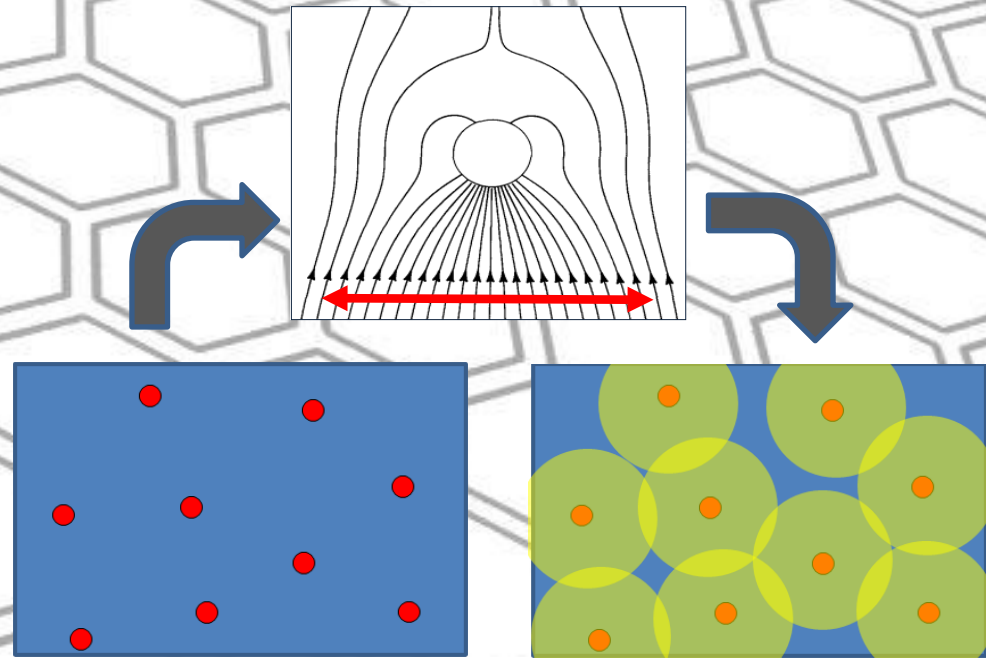
- **1% content \Rightarrow 99% effect**
 - conductive CNT networks
 - graphene gas barriers
 - resonance enhanced coupling



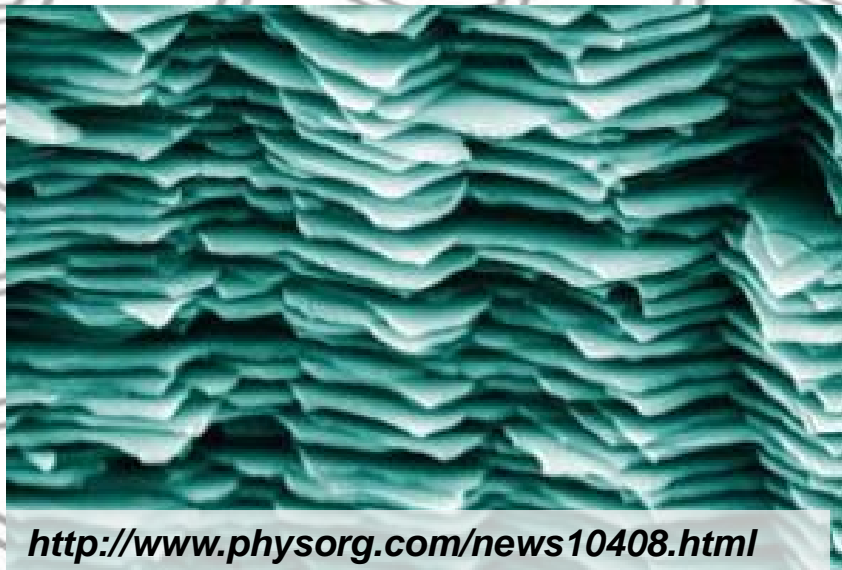
~25,000 times
volume ratio

•Two origins

- Geometric dimensionality
(1D networks in 3D, 2D
barriers, etc.)
- Resonance, field
modification, periodicity &
coherent wave effects



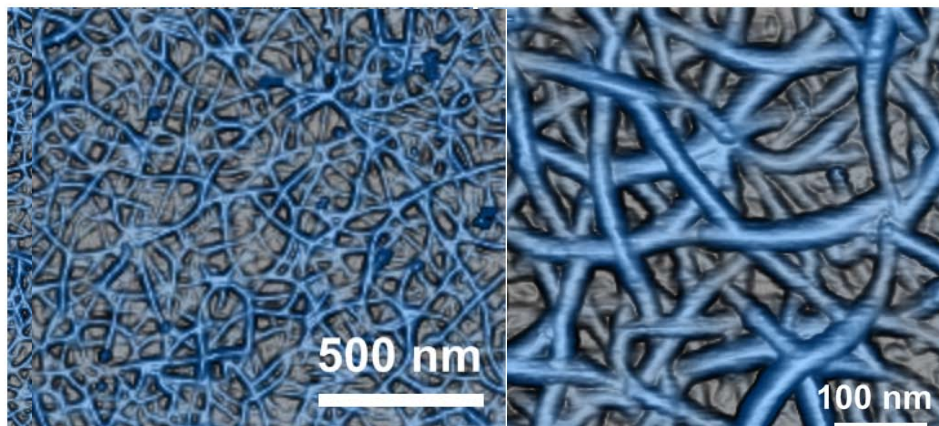
Nanoarchitectures: Percolated Networks & Stacked Platelets



- Low degree of architectural order
- Distinctive properties dictated by average proximal connection between nano-objects

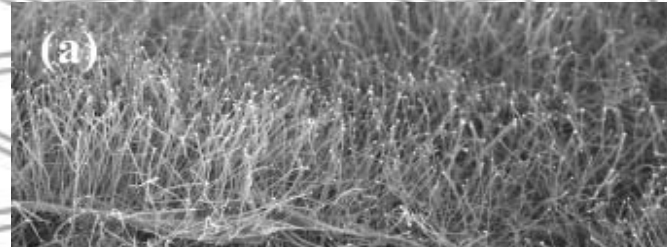
- Percolated networks:
 - Field transmission (electrical, thermal, mechanical stress)

- Stacked platelets:
 - Tortuosity (molecular permeability, crack propagation,)
 - Overlap provides property propagation (e.g. Conductivity)



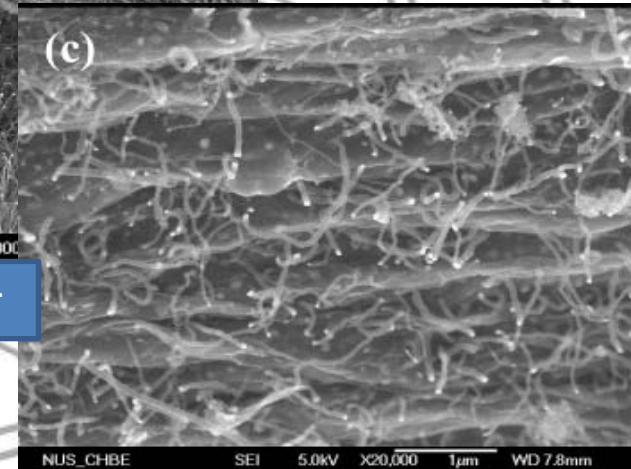
Nanoarchitectures: Pillars & Layers

- “Pillared graphene”
 - High Strength
 - High Conductivity (electrical & thermal)
 - High surface area



NUS_CHBE SEI 5.0kV X5,000

10.1021/nn102308r



NUS_CHBE SEI 5.0kV X20,000 1μm WD 7.8mm

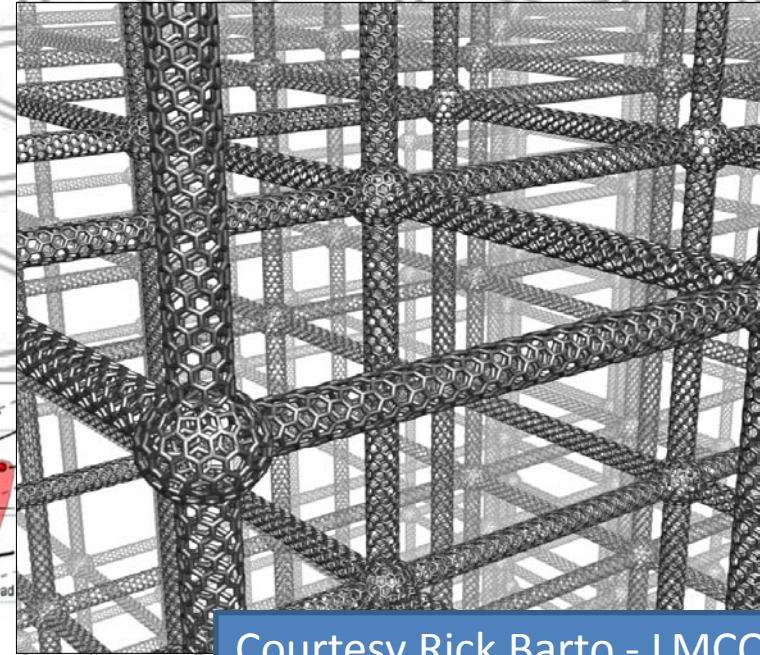
- Structural Energy Storages
 - Hydrogen Storage
 - Battery & Supercapacitor Electrodes

10.1021/nl801417w

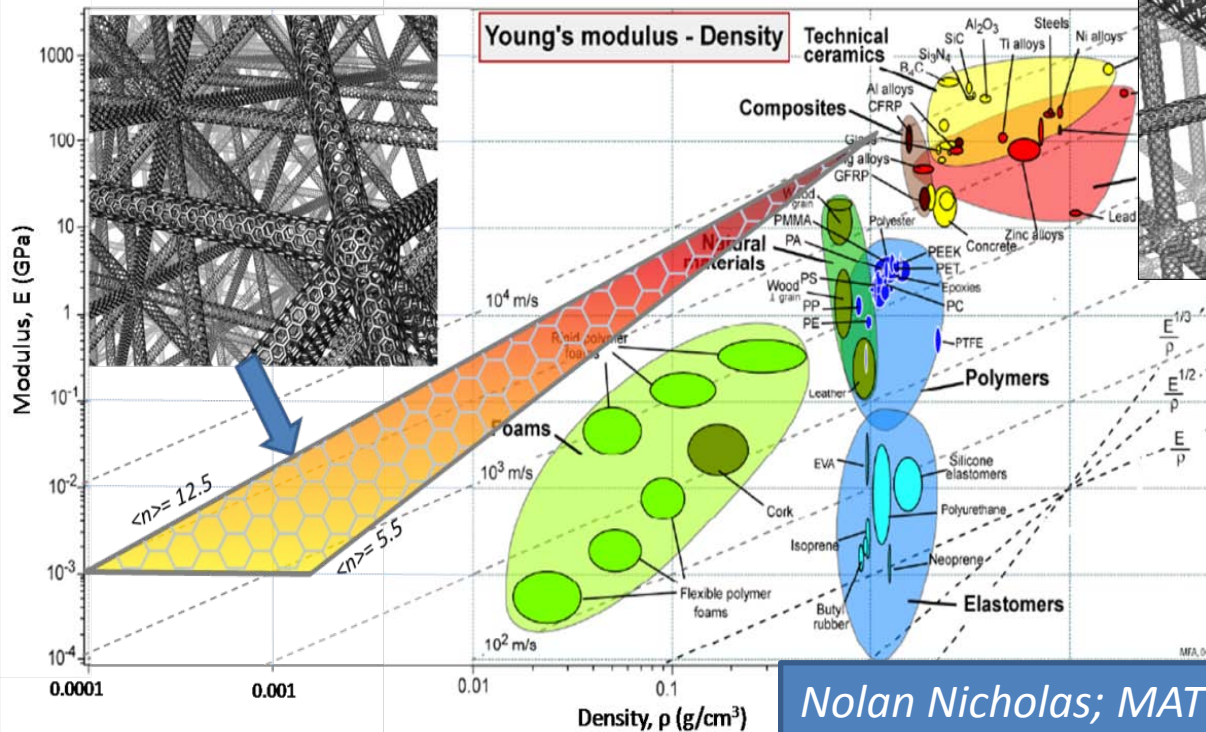
Nanoarchitectures: Spacefilling Frames

•Spaceframe

- Architecturally driven properties
- Decoupled variables
- High surface area
- Large free volume



Courtesy Rick Barto - LMCO



- Structural Energy storage
- Structural actuator materials
- Continuously graded materials (e.g. Stiff to soft)

Decoupled Variables vs. Fortuitously Coupled Variables

- Fortuitously coupled variables: you get what you get – hopefully you like it

- The key issue is how to recognize when such couplings are present

- Decoupled variables: menu item selection...

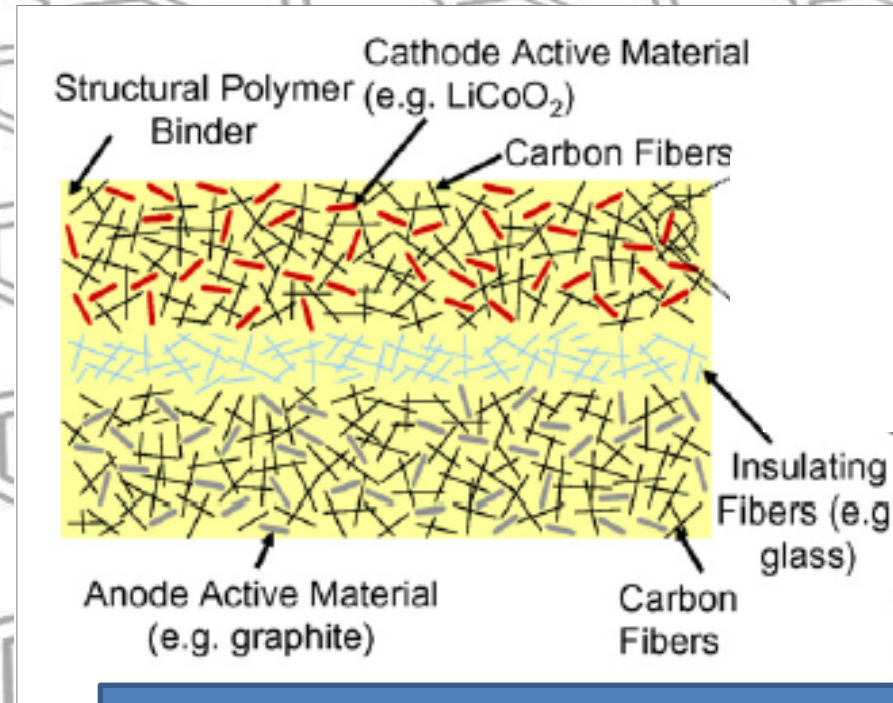
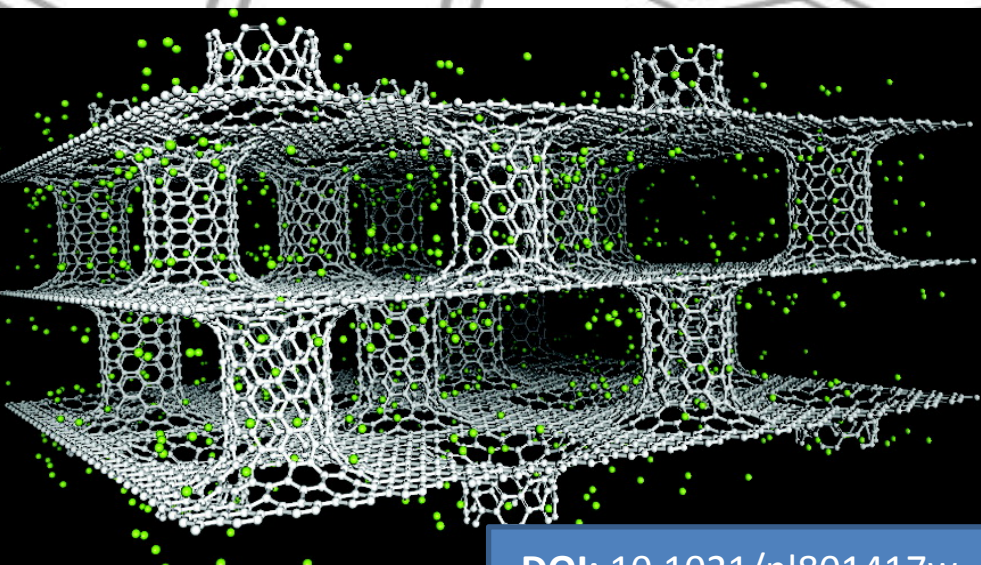
- The key is how to optimize a multidimensional parameter problem

Example Systems & Opportunities

- “Mechanical Plus”
 - Electrical Conductivity (both highly conductive and static bleed)
 - Thermal Conductivity
 - Sensor
 - Energy Harvesting/Storage
 - Vibration Damping
 - Gas Barrier
- Actuation & “Smart” Materials
- Environmentally Responsive & “Smart” Materials
- BioMedical Materials
- Epoxy Curing & Adhesive Interfaces
- Graded Materials
- Damage Protection (thermal, chemical, UV, etc.)

Structural Energy Storage

- Aircraft fuel fractions around 30% are typical of modern jet aircraft
- 19.7% of weight “around town” Nissan Leaf electric car is in its power system

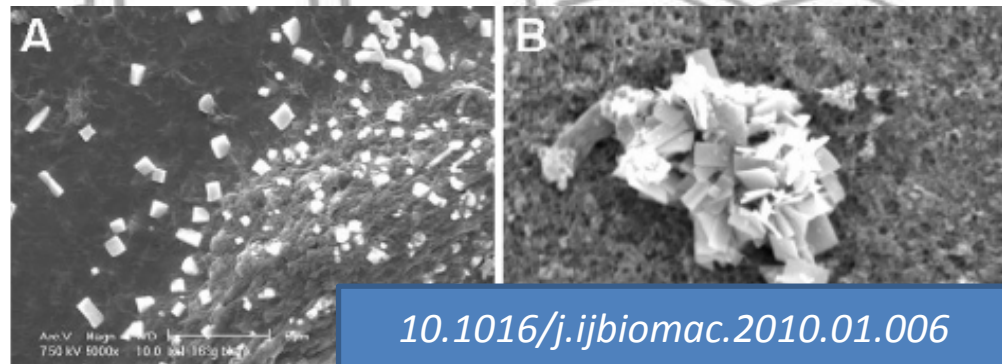
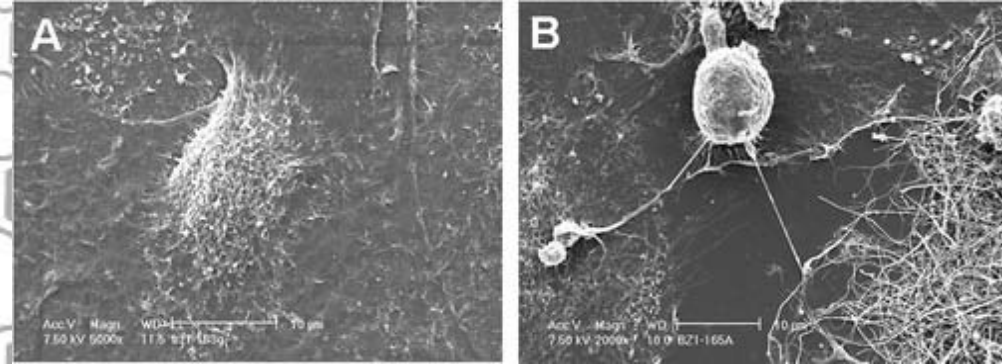


doi:10.1016/j.jpowsour.2008.09.082

BioMedical Materials

- High Strength
- Enhanced Biocompatibility
- Therapeutic Delivery

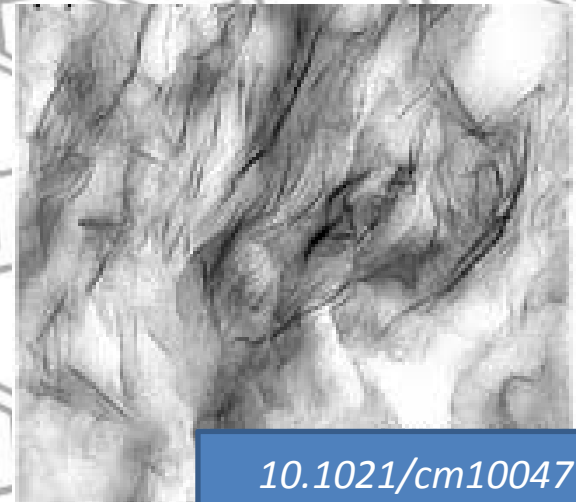
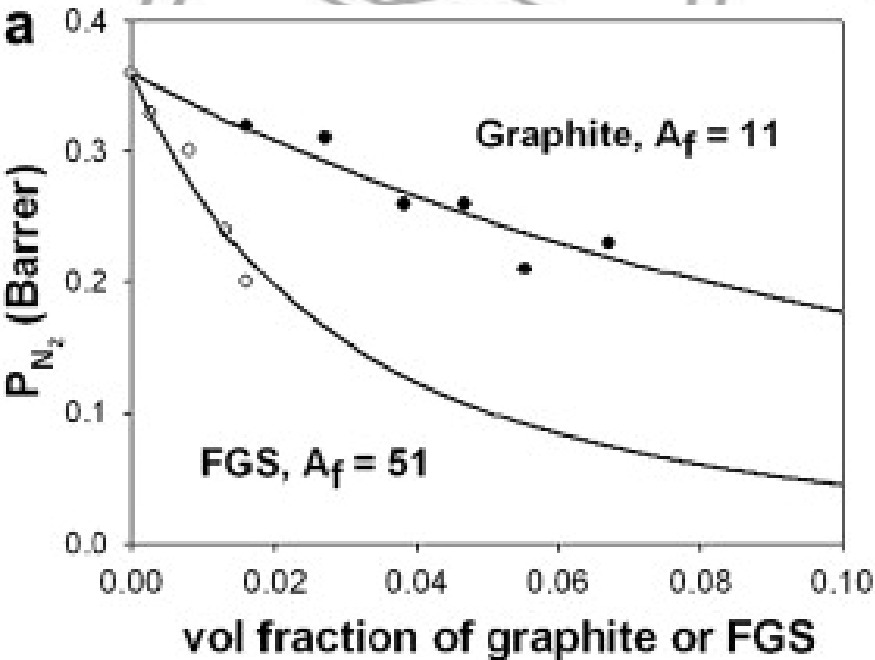
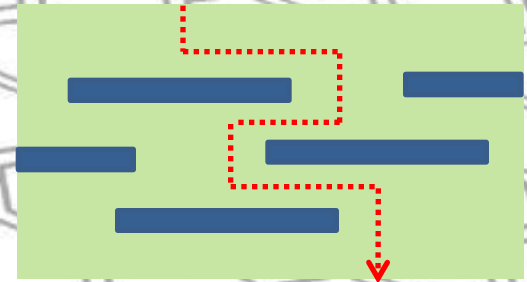
- Drug Release Materials
 - graphene oxide
 - nanodiamond
- Biocompatible implants & scaffolds



Gas Barrier

Graphene Nanocomposite Gas Barrier

- Graphene impermeability
- Nanoplatelet tortuosity
- Material Stress Field & Gas Solubility



10.1021/cm100477v

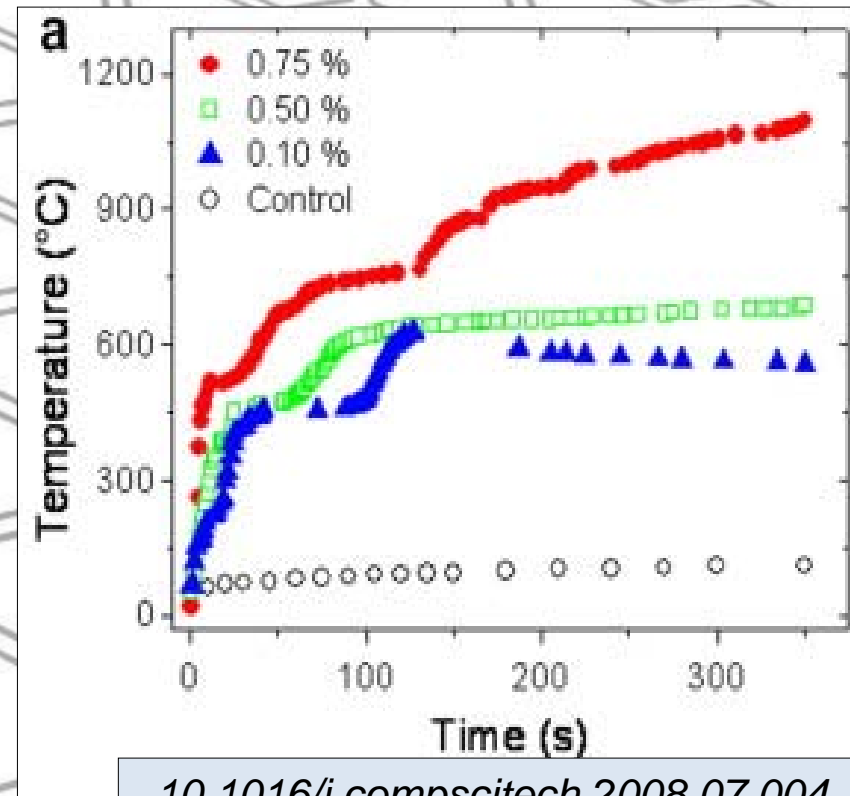
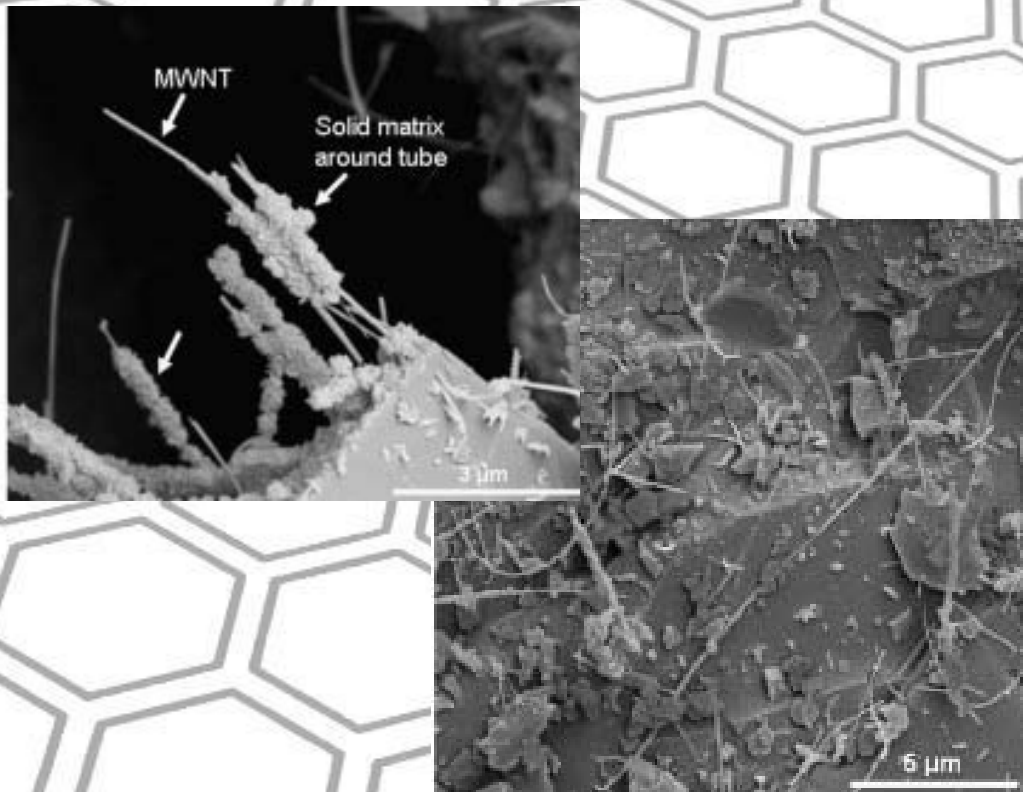
Simultaneous enhancements in

- Mechanical Strength
- Electrical & Thermal Conductivity
- In-Situ Sensing

10.1016/j.polymer.2009.05.038

Epoxy Curing

Improved strength
Enhanced curing

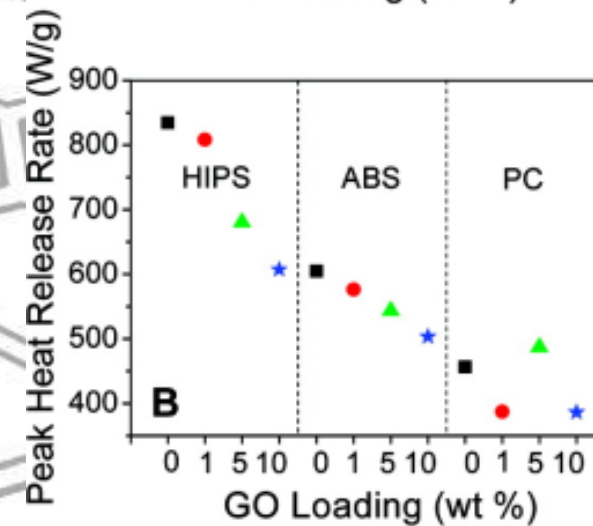
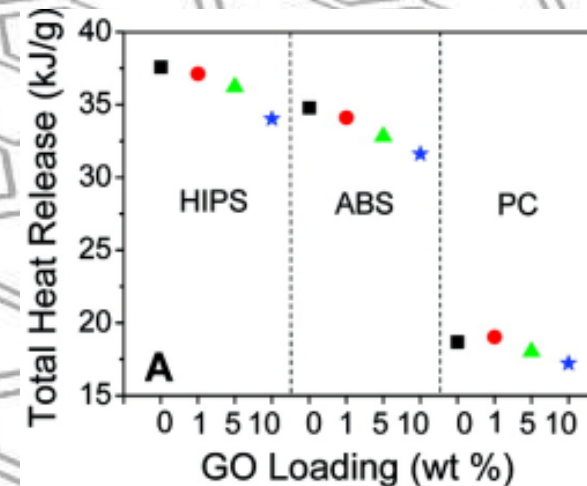
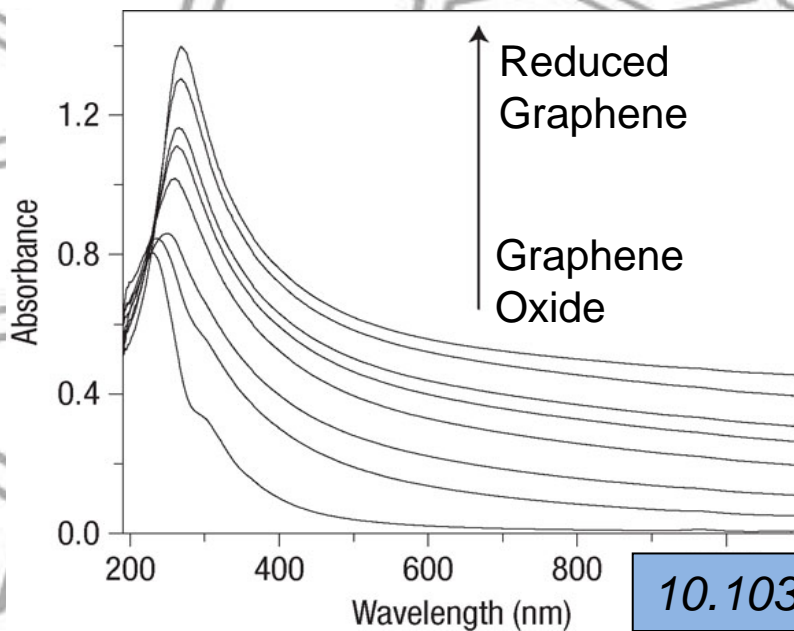


10.1016/j.compscitech.2008.07.004

Nanocomposite Protection

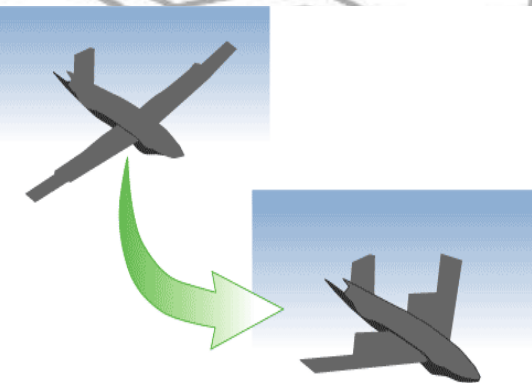
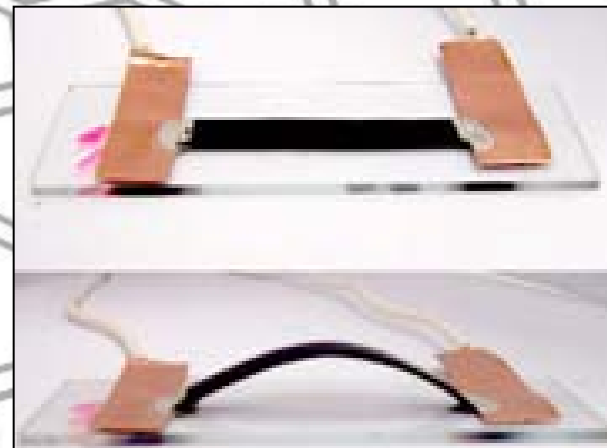
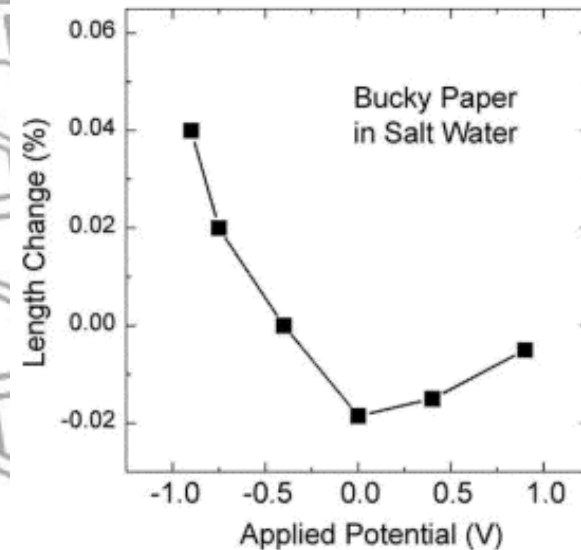
Chemical & physical properties of graphenic carbon engender protective properties to a polymer matrix while also providing mechanical enhancements

- Fire Retardancy
- UV Absorbance
- Chemical Attack Resistance



Actuators & Smart Materials

- Smart/adaptive materials provide adaptive multifunctionality
- CNTs have been observed to have extraordinarily high electro-actuation properties
- Adaptive thermal-conductivity nanomaterials could provide passive optimization of clothing & device insulation

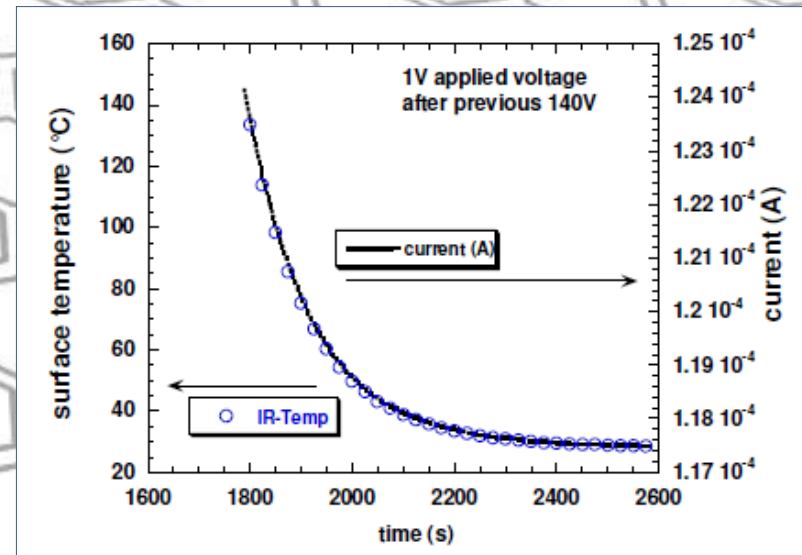


In-Situ Sensors

Mechanical Enhancement

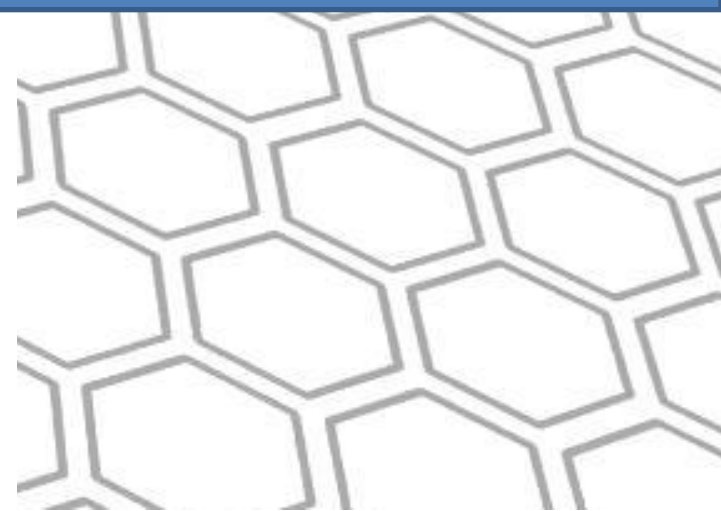
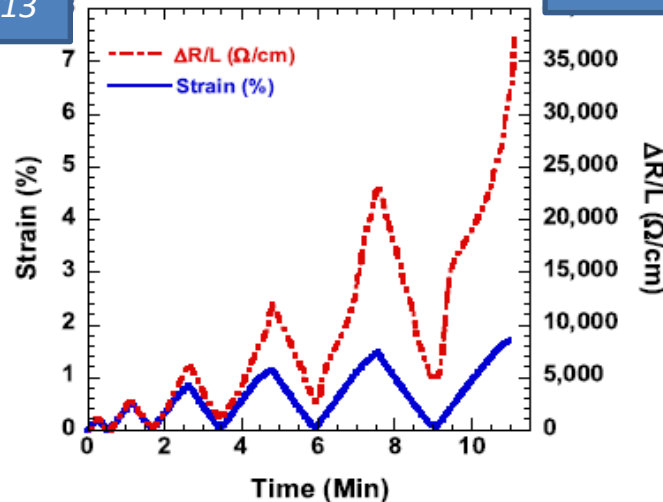
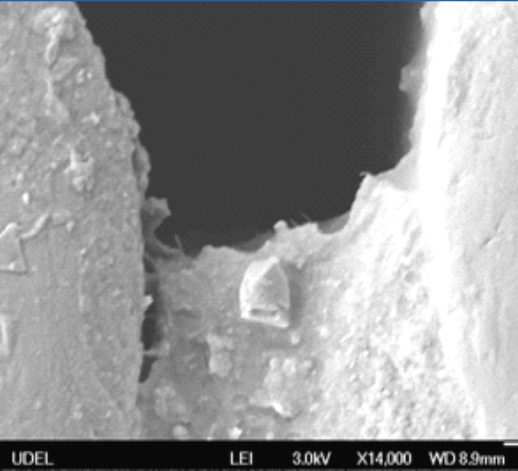
In-Situ Sensors

- CNT composite conductivity is often sensitive to operating conditions
 - Strain
 - Temperature



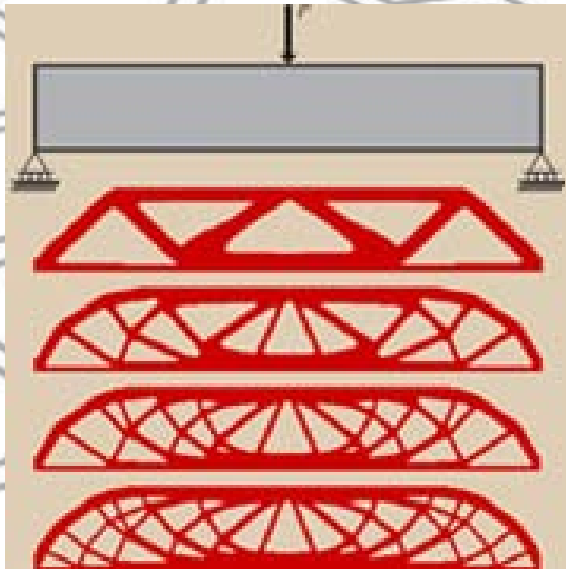
10.1088/0957-4484/19/21/215713

ICCE-17 Proc.; Neitzert, et al. 20733.pdf

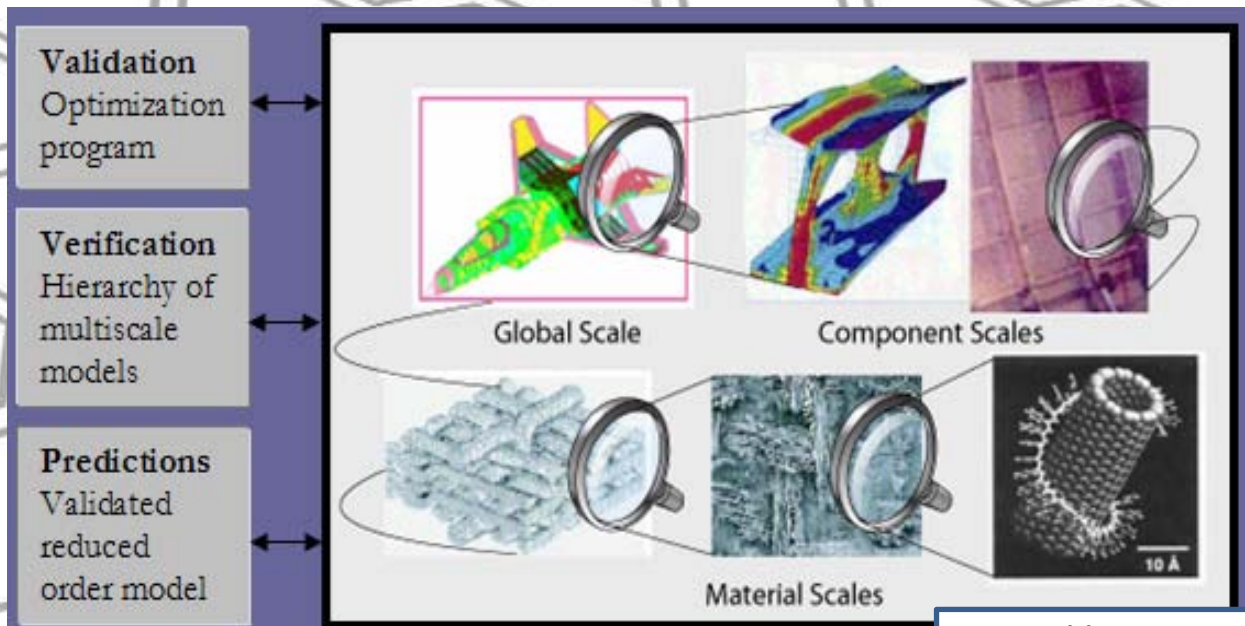


Achieving Multifunctionality: Multi-Property Optimization

- Topological optimization
- Integrated system optimization
- Weighted optimization problem in multidimensional space



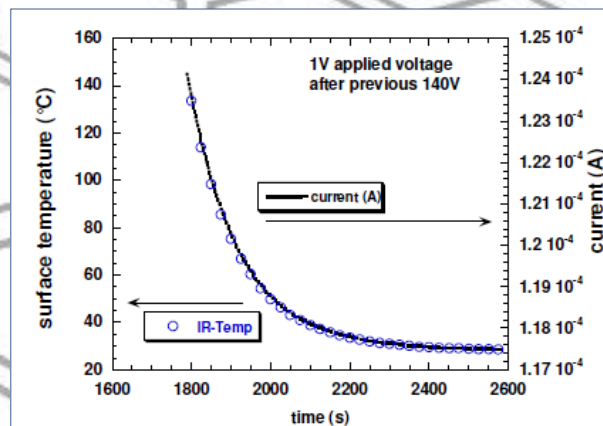
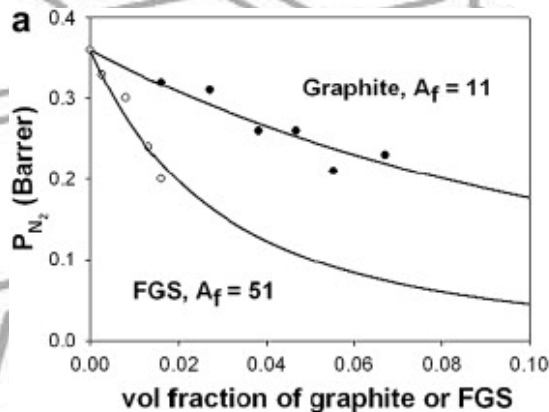
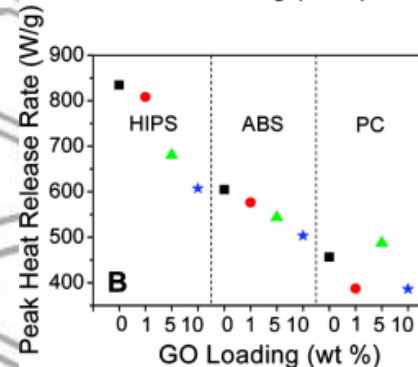
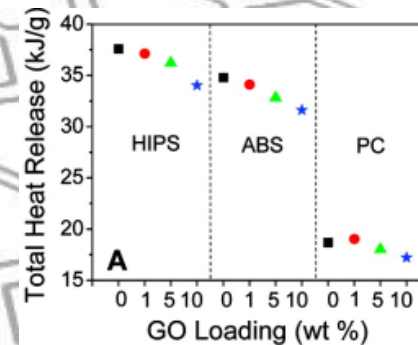
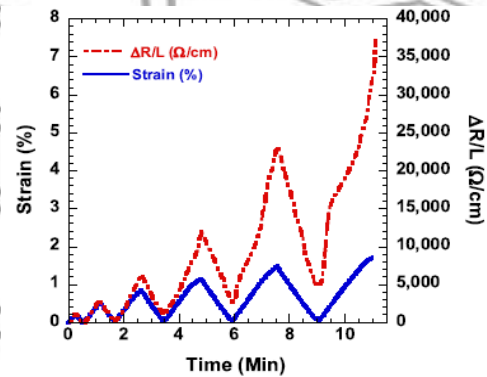
<http://www.civil.jhu.edu/research-highlights>



<http://feos.biz/>

Achieving Multifunctionality: Multiparameter Measurement

- Materials systems & properties are measured as independent, uncorrelated data points
- Integral correlation & regularization of multiparameter testing is needed



About MATRIC

MATRIC is a 501(c)(3) non-profit research and development corporation

- Reinvest earnings in new research
- Expertise in R&D commercialization from ideation through production
- Offices in Charleston (WV), Morgantown (WV) and Oak Ridge (TN)

•**Expertise in**

- Biomass fuels & products
- Fossil fuels & products
- Environmental technologies
- Polymer synthesis & processing
- Nanomaterials
- Separations technologies
- Catalysis
- Agricultural Sciences
- Biomedical Device Development
- Cellular & Immunological Research
- Aerospace Software & Systems Engineering

