# CENTER FOR HIERARCHICAL MATERIALS DESIGN

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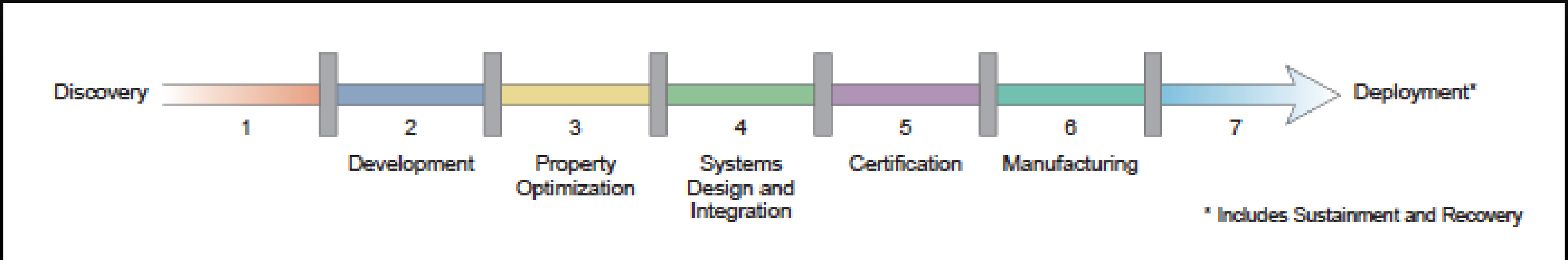
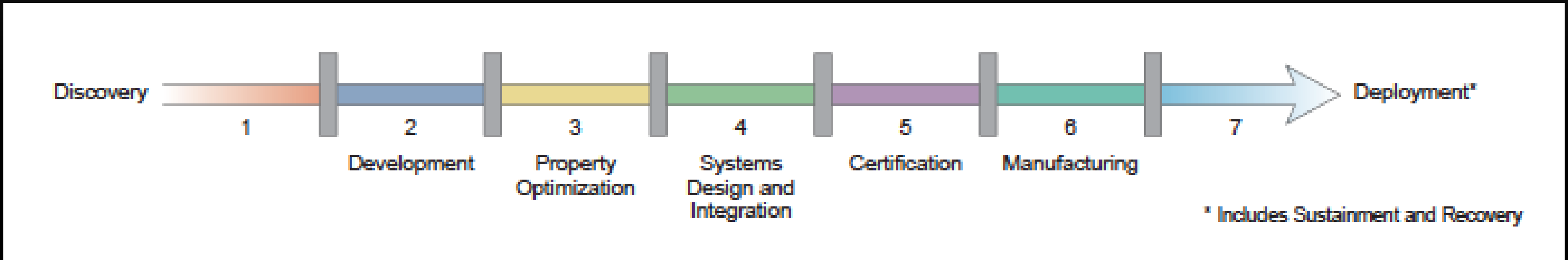
# MATERIALS DEVELOPMENT




This is a very long and arduous (expensive) process:

- It typically requires 10-20 years to insert new materials in an application
- Example:  it took 20 years to move Li-ion batteries from discovery to marketplace. Still ongoing today: automotive batteries

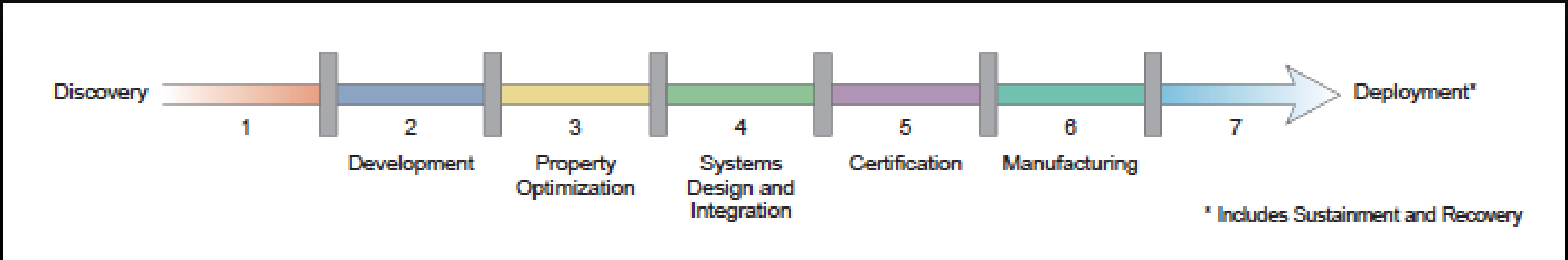
# MATERIALS DEVELOPMENT




Reason:

- Intuitive development of new materials
- Trial and error experimentation
- Inability to predict material properties for a given composition and processing sequence

# MATERIALS DEVELOPMENT




Solution:

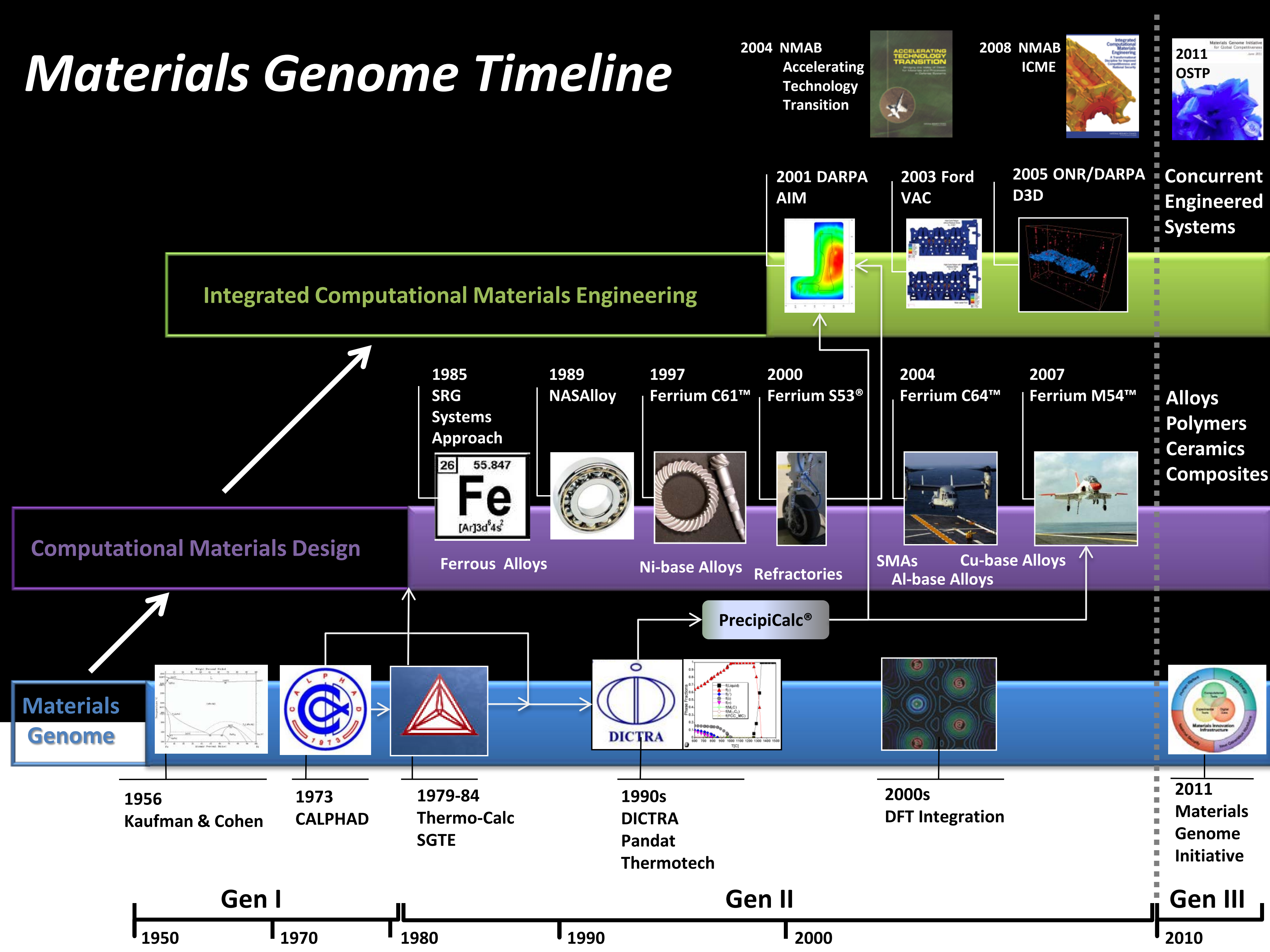
- Integrate computations, experimental tools, and digital data to speed up the design process

# **Materials Genome Initiative**
## for Global Competitiveness

June 2011

Fundamental databases and tools enabling reduction of the 10-20 year materials creation and deployment cycle by 50% or more

**National Science and Technology Council (NSTC)/ Office of Science and Technology Policy (OSTP)**


Materials Genome Timeline
2004 NMAB Accelerating Technology Transition
2008 NMAB ICME
2011 OSTP
2001 DARPA AIM
2003 Ford VAC
2005 ONR/DARPA D3D
Concurrent Engineered Systems
Integrated Computational Materials Engineering
1985 SRG Systems Approach
1989 NASAlloy
1997 Ferrium C61™
2000 Ferrium S53®
2004 Ferrium C64™
2007 Ferrium M54™
Alloys
Polymers
Ceramics
Composites
26 55.847 Fe [Ar]3d⁶4s²
Computational Materials Design
Ferrous Alloys
Ni-base Alloys
Refractories
SMAs
Cu-base Alloys
Al-base Alloys
PrecipiCalc®
Materials Genome
DICTRA
1956 Kaufman & Cohen
1973 CALPHAD
1979-84 Thermo-Calc SGTE
1990s DICTRA Pandat Thermotech
2000s DFT Integration
2011 Materials Genome Initiative
Gen I
Gen II
Gen III
1950
1970
1980
1990
2000
2010

# NIST CENTER OF EXCELLENCE IN ADVANCED MATERIALS

- Center for Hierarchical Materials Design: CHiMaD
- $5 million per year
- Organizations involved:

THE UNIVERSITY OF CHICAGO

NORTHWESTERN UNIVERSITY

Argonne NATIONAL LABORATORY

QUESTEK INNOVATIONS LLC

ASM INTERNATIONAL The Materials Information Society

FAYETTEVILLE STATE UNIVERSITY

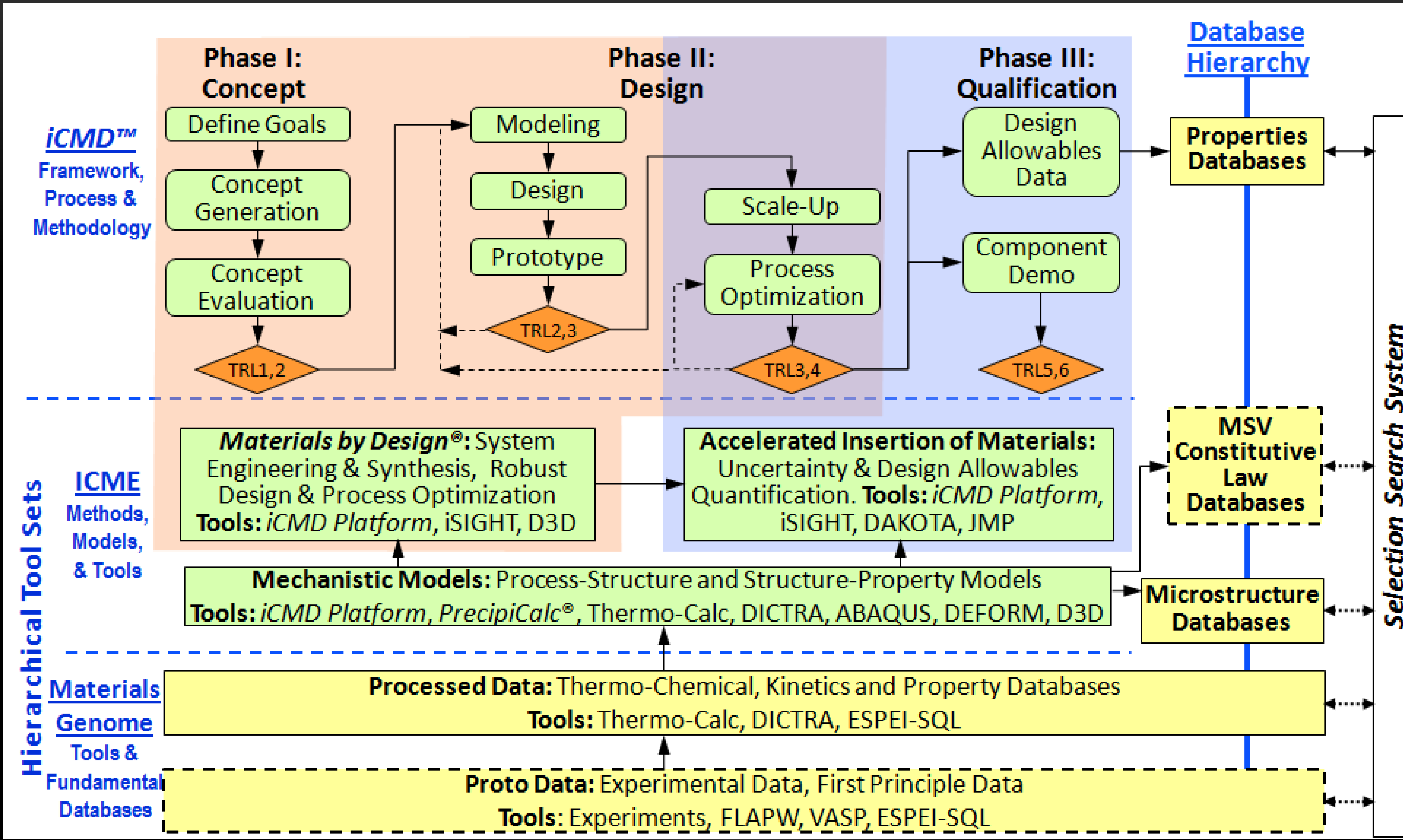
- Co Directors: Greg Olson (Northwestern), Juan DePablo (University of Chicago)

# OBJECTIVES OF CHIMAD

- Create a collaborative environment and concentration of scientific and technical capability to accelerate materials discovery and development
- Provide opportunities to transition new breakthroughs in advanced materials to industry
- Convene multidisciplinary and multi-sector communities for in-depth discussions
- Provide training opportunities for scientists and engineers in materials metrology
- Foster the development of integrated computation, modeling and data-driven tools
- Foster the discovery of new materials
- Establish opportunities for extended collaborations with NIST

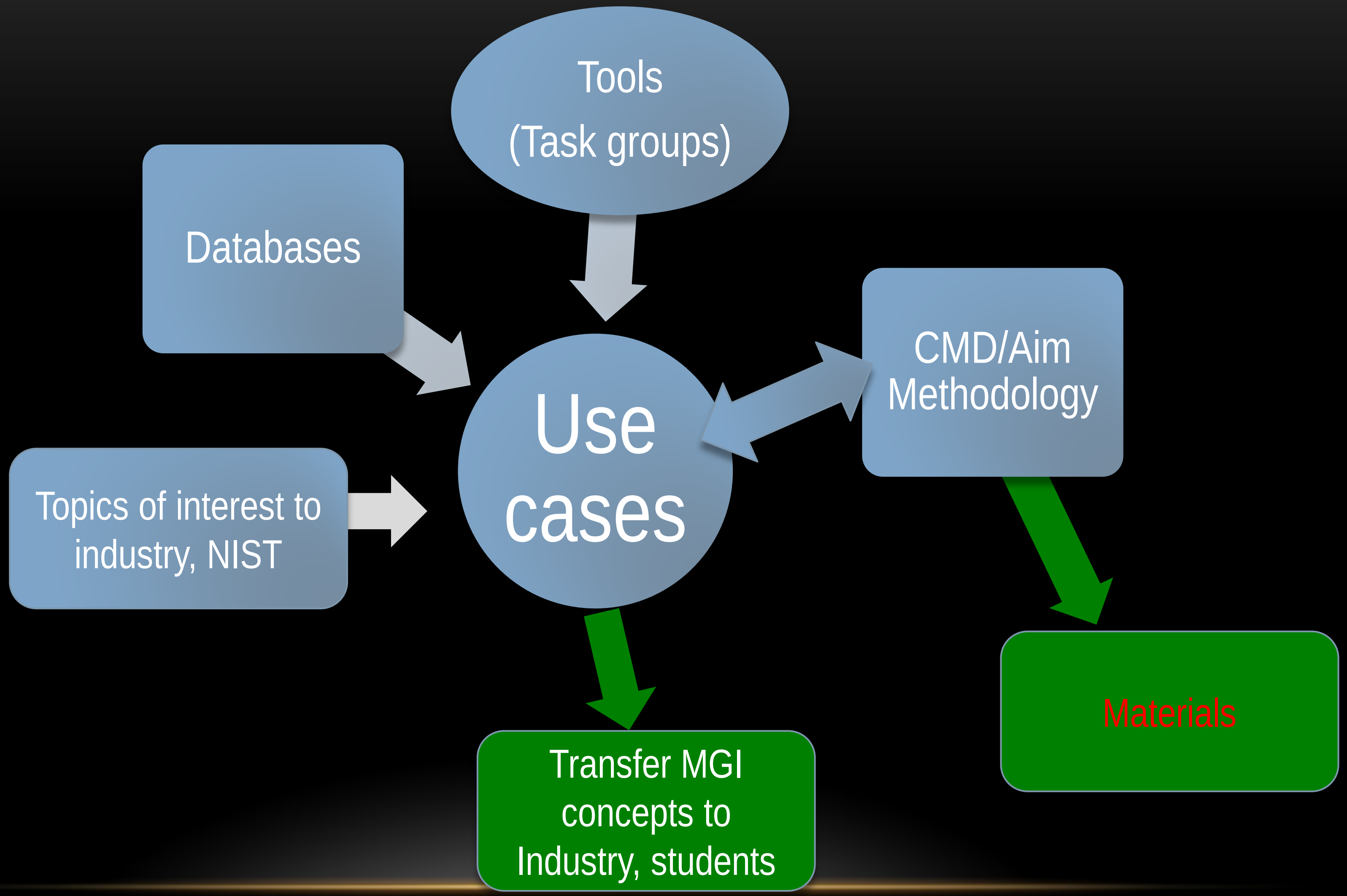
# HOW CAN WE ACCOMPLISH THESE GOALS?

- Leverage our long history of materials design and collaborative research
- Use Case Groups
  - focus on particular materials of industrial and scientific importance
  - involve industrial collaborators
  - transfer the design methodology to industry and other stakeholders
- Tool development
  - Develop community standard codes for both hard and soft materials design
  - Develop materials databases that are motivated by topics of the use groups
  - Develop experimental methods for rapid assessment of materials properties
- Convene workshops on issues that are central to the implementation of the MGI
- Interact closely with NIST

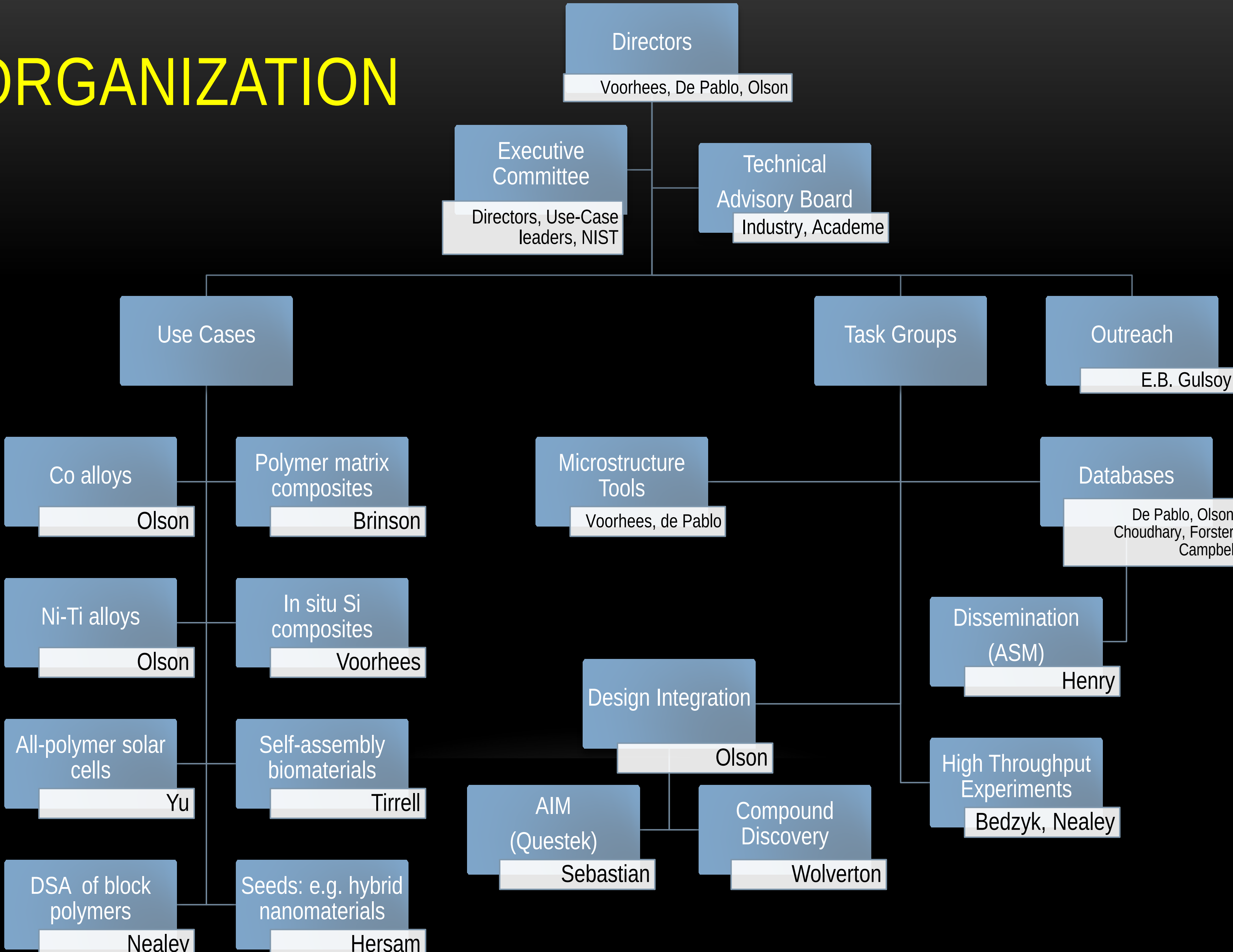


Phase I: Concept
Phase II: Design
Phase III: Qualification
Database Hierarchy
iCMD™
Framework, Process & Methodology
Define Goals
Concept Generation
Concept Evaluation
TRL1,2
Modeling
Design
Prototype
TRL2,3
Scale-Up
Process Optimization
TRL3,4
Design Allowables Data
Component Demo
TRL5,6
Properties Databases
Selection Search System
Hierarchical Tool Sets
ICME
Methods, Models, & Tools
Materials by Design®: System Engineering & Synthesis, Robust Design & Process Optimization
Tools: iCMD Platform, iSIGHT, D3D
Accelerated Insertion of Materials: Uncertainty & Design Allowables Quantification. Tools: iCMD Platform, iSIGHT, DAKOTA, JMP
MSV Constitutive Law Databases
Mechanistic Models: Process-Structure and Structure-Property Models
Tools: iCMD Platform, PrecipiCalc®, Thermo-Calc, DICTRA, ABAQUS, DEFORM, D3D
Microstructure Databases
Materials Genome
Tools & Fundamental Databases
Processed Data: Thermo-Chemical, Kinetics and Property Databases
Tools: Thermo-Calc, DICTRA, ESPEI-SQL
Proto Data: Experimental Data, First Principle Data
Tools: Experiments, FLAPW, VASP, ESPEI-SQL

# IMPLEMENTATION



# ORGANIZATION



# DATABASES

- Will contain CALPHAD protodata: tie lines, thermochemical data, elastic constants, as well as higher level data such as interfacial energies
- Start with metals relevant to the work group projects, and then extend to soft materials
- Standardized metadata describing error estimates that are needed in incorporation into higher level CALPHAD databases
- Unlike assessed CALPHAD databases, which can be proprietary, this will be open
- Thus, we hope to make this a repository for information on new systems in the future
- Statistical learning can be applied to this database to aid in material discovery
- Perhaps incorporate the Open Quantum Mechanical database

# OUTREACH

- ASM Action in Education Committee,  Materials Genome Toolset dissemination to materials UG programs
- Integration in NU ICME MS and Predictive Science & Engineering Design (PSED) doctoral programs
- Workshops with the community:
  - Databases: standards, coordination and composition
- First workshop at NIST:
  - Database development
- A MGI seminar series broadcast to NIST, jointly hosted by Northwestern, the University of Chicago, and Argonne
- Summer schools
- Yearly TAB meetings

# TOOLS

- Evolutionary Strategies (design of microstructure)
- Theoretically Informed Coarse Grained (TICG) Models
- Prediction of GISAXS, SAXS
- Community standard phase field code
- High throughput experiments and calculations

# Cobalt Alloy Design

**G. Olson (NU)**, D. Dunand (NU), D. Seidman (NU), P. Voorhees (NU),
M. Stan (NAISE, ANL) C. Wolverton (NU)

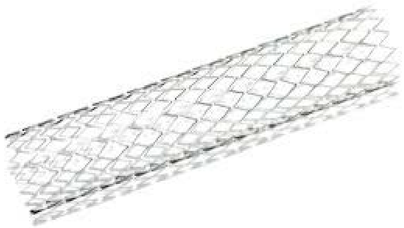
- Motivation:
  - Need turbine blade alloys that exceed the use temperatures of Ni-based superalloys
  - Wear resistant ambient temperature applications to replace Be-Cu
- Goals:
  - Near-term: Ambient temperature bushing alloy
  - Long-term: High-temperature aeroturbine superalloy

Center for Hierarchical Materials Design
CHiMaD

# Nanodispersion-Strengthened Shape Memory Alloys

**G. Olson (NU)**, D. Dunand (NU),W-K. Liu (NU)  D. Seidman (NU), A. Umantsev (FS), C. Wolverton (NU)

- Motivation:
  - Widely used in medical, aerospace and automotive sectors
  - Current alloys are susceptible to instability after many cycles



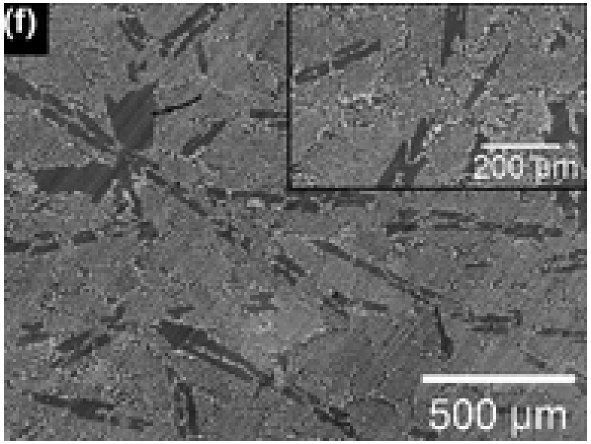
- Goals:
  - Near-term: Pd-stabilized alloys for medical devices
  - Long-term: High-temperature aeroturbine superalloy


CHiMaD

# In-Situ Si Composite Materials

**P. Voorhees (NU)**, J. De Pablo (UC), W. Chen (NU), S. Davis (NU) , C. Wolverton (NU)

- Motivation:
  - Corrosion resistant, tough alloys
  - Avoid the complications of classical ceramic processing, such as sintering
  - Employ insitu Si-composites
- Goals:
  - Near-term: A multicomponent eutectic growth model
  - Long-term: A tough, castable Si alloy




$Si$-$CrSi_2$ composite

(Fischer and Schuh, J. Am Ceram. Soc, 2012)

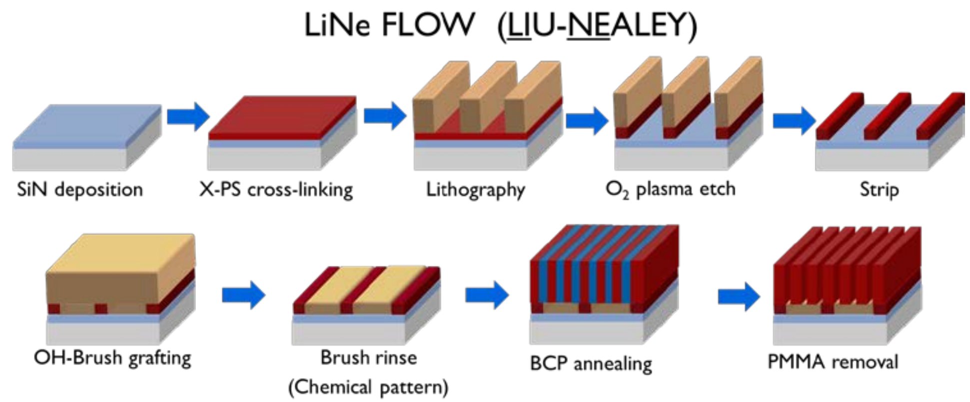
# Directed Self-Assembly of Block Polymers

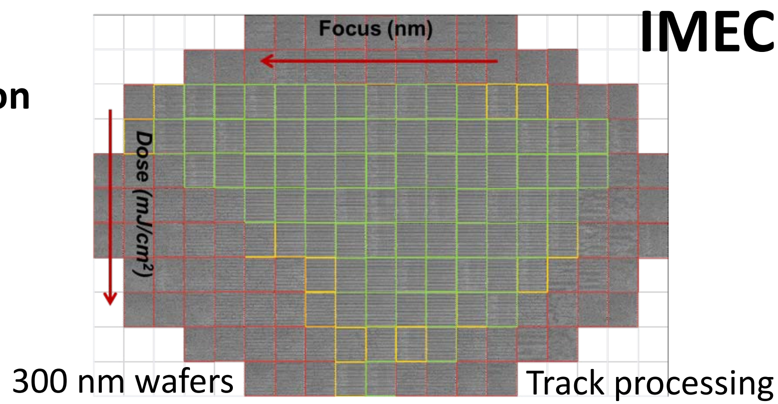
**P. Nealey (UC),** J.J. de Pablo (UC), H. Jaeger (UC), M. Olvera de la Cruz (NU), S. Sibener (UC), L. Yu (UC)

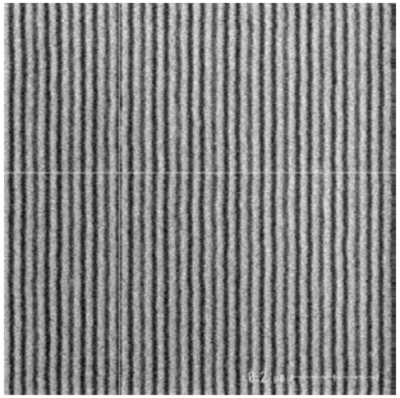
## *MOTIVATION*

### Lithography

- **Workhorse of semiconductor industry**
- **Important fraction of cost of electronic devices**
- **Need for new materials and processes for next-generation lithography**
- **Sub-10 nm patterning**
- **Need for metrology**
- **Need for design tools**



**Initial Goals:** **Robust, pilot-line validated directed self-assembly for sub 10 nm lithography**

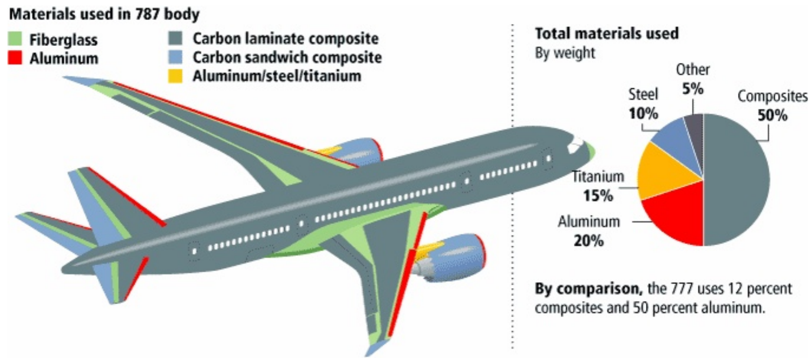
- Search for new polymers and processing techniques
- Design materials and processes
- Validate by comparison to experiment
- Develop metrology tools and advanced simulation tools for non-equilibrium assembly

# Polymer Matrix Composites

**C. Brinson (NU),** J.J. de Pablo (UC), Keten (NU), E. Luijten (NU)

## *MOTIVATION*

- **Composites are lightweight, corrosion resistant, tailorable, low cost**
- **Limited understanding of:**
  **- multiphase composite properties**
  **- simultaneous control of electrical/mechanical properties**
  **- long-term properties and durability under use conditions**




**Initial Goals: Comprehensive design of composite materials**

- Control of surface-polymer interactions
- Tune thermomechanical and electric/dielectric properties
- Use of nanofillers for tuning of electrical conductivity, toughness and durability
- Multiscale prediction and design of materials with known electric, dielectric and mechanical properties

http://siag.project.ifi.uio.no/problems/grandine/Composites01.jpg

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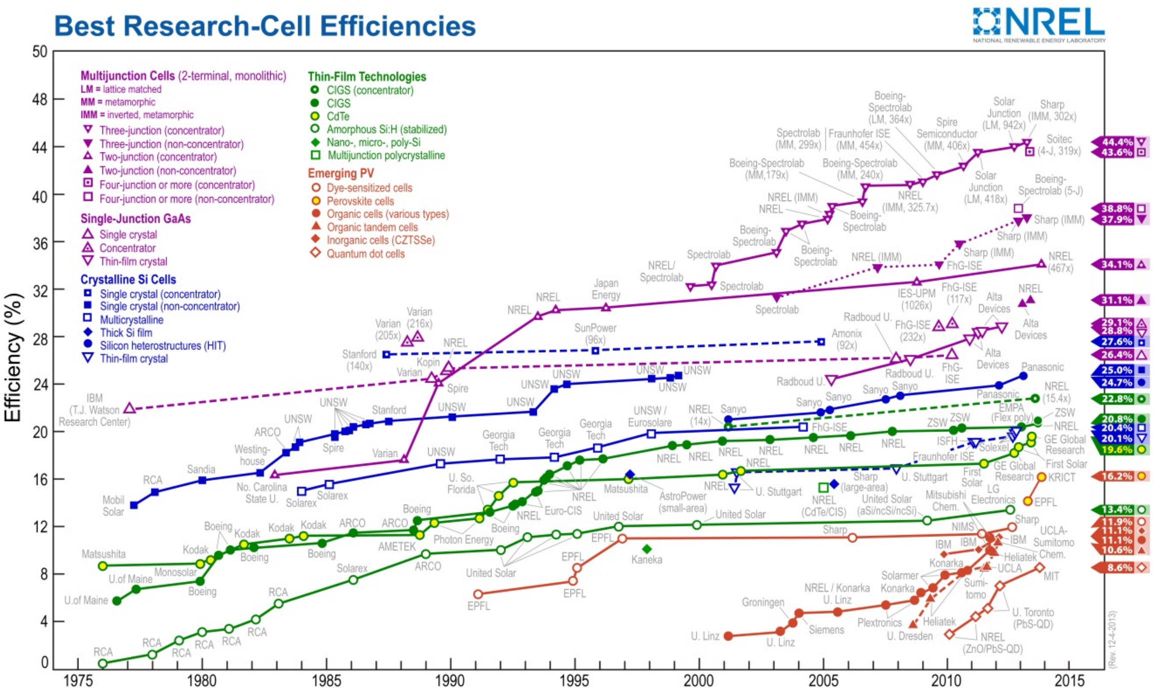
# All-Polymer Organic Solar Cells

**L. Yu (UC),** J.J. de Pablo (UC), G. Galli (UC), M. Hersam (NU), H. Jaeger (UC), M. Olvera de la Cruz (NU), M. Tirrell (UC)

## *MOTIVATION*




### Energy

- **Inorganic solar cells currently exhibit higher efficiency**
- **Rapidly improving performance of organic cells**
- **Organic cells made from earth abundant materials, light weight, stable, processing, morphology optimization**

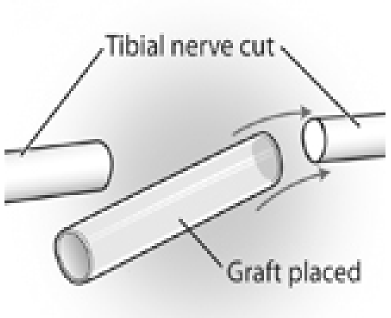
**Initial Goals: Create all organic solar cells**

- Search for new design principles for electron accepting polymers
- Generate new materials with greater potential than fullerene derivatives as n-type materials
- Novel accepting polymers w. high mobility for organic electronics

# Self-Assembly of Biomaterials

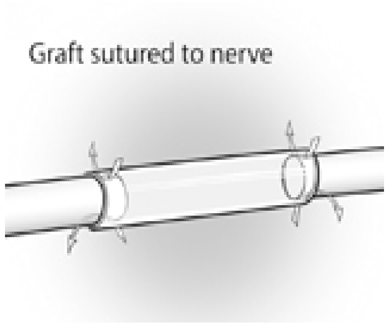
**M. Tirrell (UC),** J.J. de Pablo (UC), E. Luijten (NU), M. Olvera de la Cruz (NU), L. Yu (UC)

## *MOTIVATION*



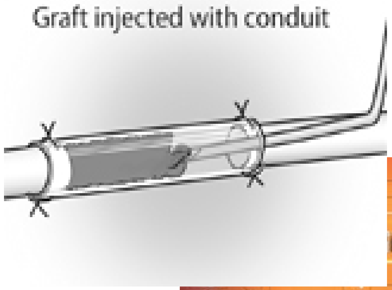

**Military**

- **Improvised explosive devices (IEDs) cause severe blast and tissue loss injuries**
- **Improved body armor has improved survival rates and increased frequency of injury to limbs/digits**




**Civilians**

- **2.8% of trauma patients have peripheral nerve damage**
- **Nerve injury costs $7 billion dollars in the US alone**
- **50,000 nerve repair procedures per year**




**Initial Goals: Create a self assembled matrix**

- Injectable
- In situ gel formation
- Stiffness in range of neural tissue
- Promote growth and activity of Schwann cells

# Seed Groups

- Solution processed nanomaterials and heterostructures: M. Hersam (NU), T. Marks (NU), Yu (UC), Galli (UC)
- Non-planar heterostructures: L. Lauhon (NU)
- Deformation processing: J. Caio (NU)

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