Center for Hierarchical Materials Design

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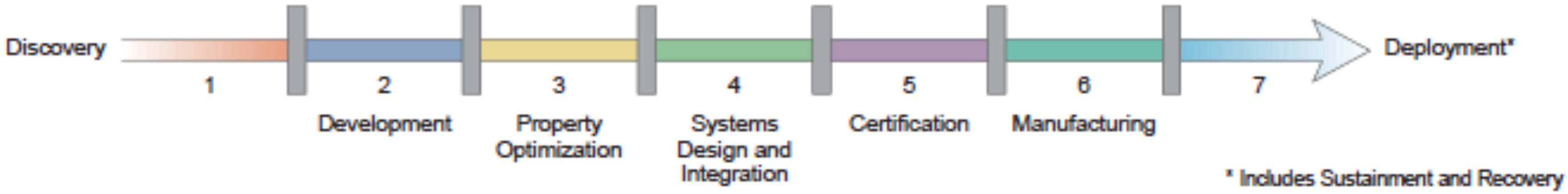
CHiMaD

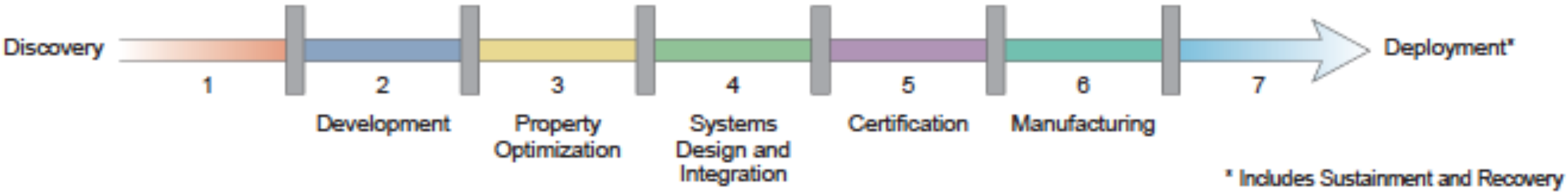
Materials Development



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



Discovery

1

2 Development

3 Property Optimization

4 Systems Design and Integration

5 Certification

6 Manufacturing

7

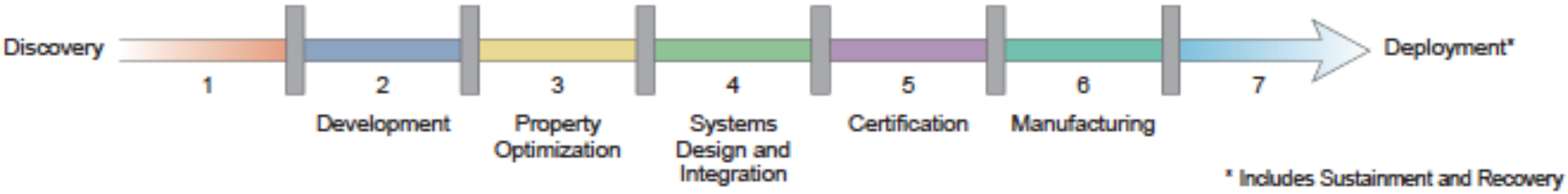
Deployment*

* Includes Sustainment and Recovery

Reason

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

Materials Development



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Solution

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

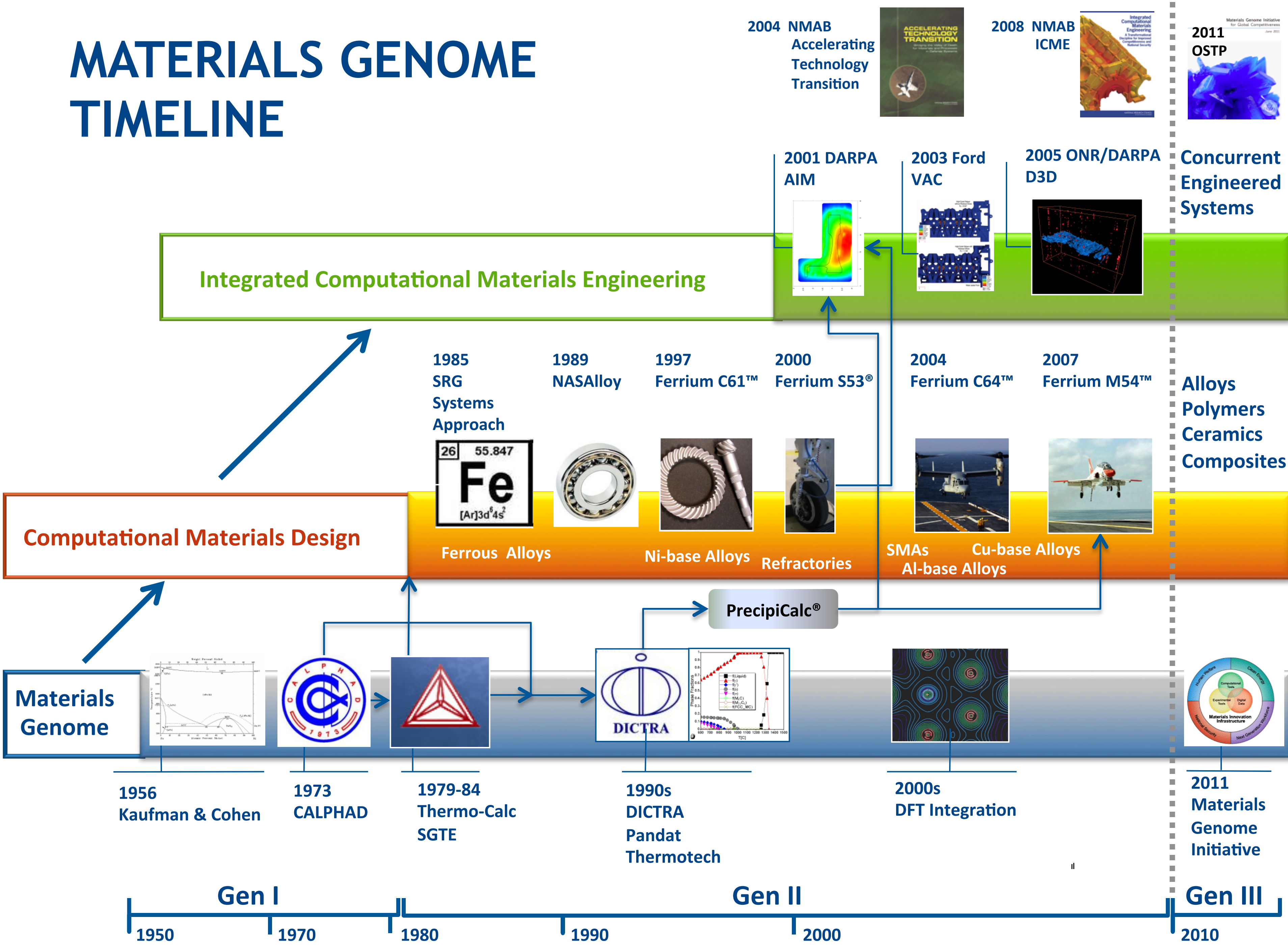
Materials Genome Initiative for Global Competitiveness

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

Integrated Computational Materials Engineering

2001 DARPA AIM

2003 Ford VAC

2005 ONR/DARPA D3D

Concurrent Engineered Systems

Computational Materials Design

1985 SRG Systems Approach

1989 NASAlloy

1997 Ferrium C61™

2000 Ferrium S53®

2004 Ferrium C64™

2007 Ferrium M54™

Alloys
Polymers
Ceramics
Composites

Ferrous Alloys

Ni-base Alloys

Refractories

SMAs

Al-base Alloys

Cu-base Alloys

PrecipiCalc®

Materials Genome

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

NIST Center for Excellence in Advanced Materials

- Center for Hierarchical Materials Design (CHiMaD)
- Chimad.northwestern.edu

Co-directors:
Greg Olson (Northwestern University), Juan De Pablo (University of Chicago)

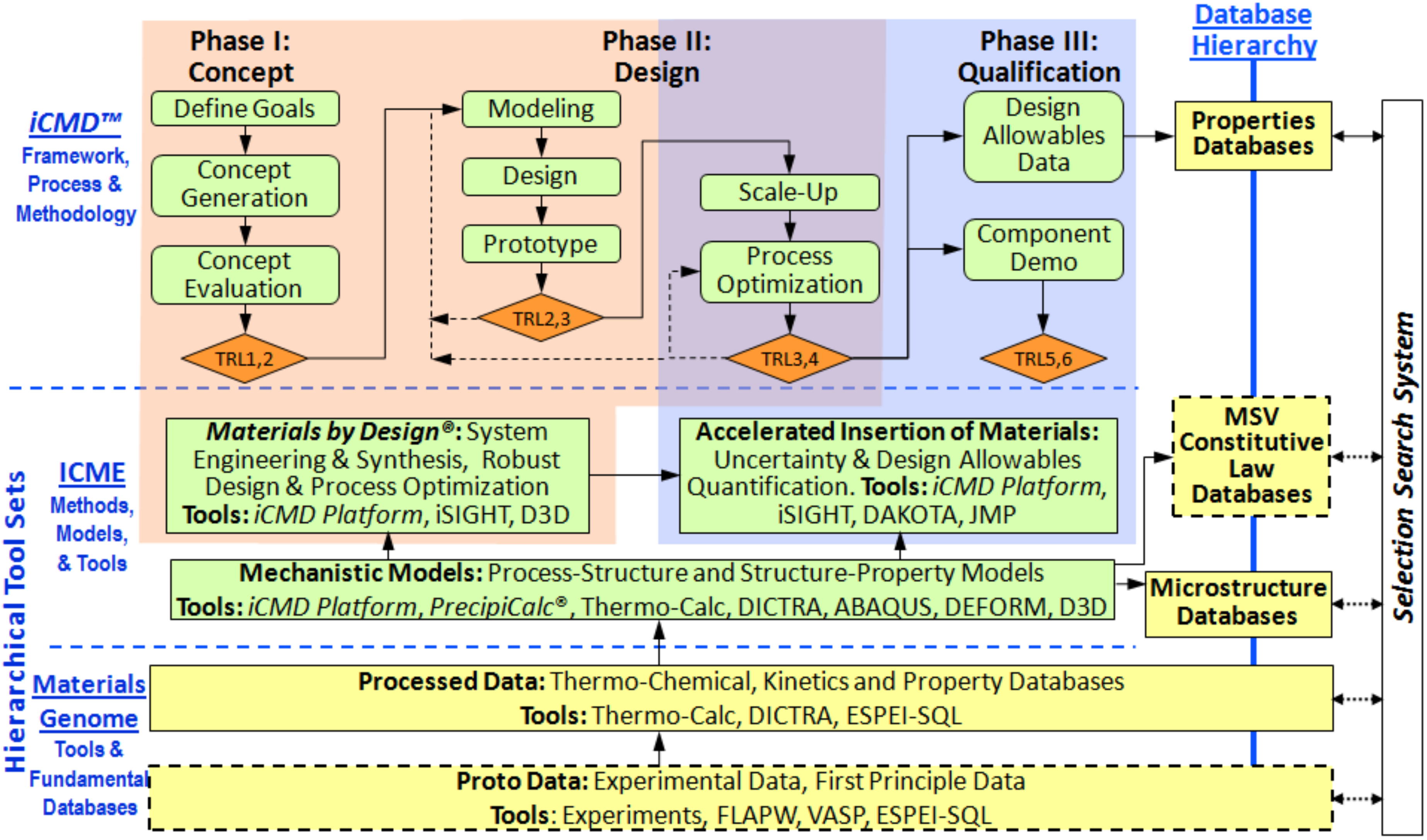
CHiMaD

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

- Define Goals
- Concept Generation
- Concept Evaluation
- TRL1,2

Phase II: Design

- Modeling
- Design
- Prototype
- TRL2,3
- Scale-Up
- Process Optimization
- TRL3,4

Phase III: Qualification

- Design Allowables Data
- Component Demo
- TRL5,6

Database Hierarchy

- **Properties Databases**
- **MSV Constitutive Law Databases**
- **Microstructure Databases**

Selection Search System

Hierarchical Tool Sets

iCMD™ **Framework, Process & Methodology**

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

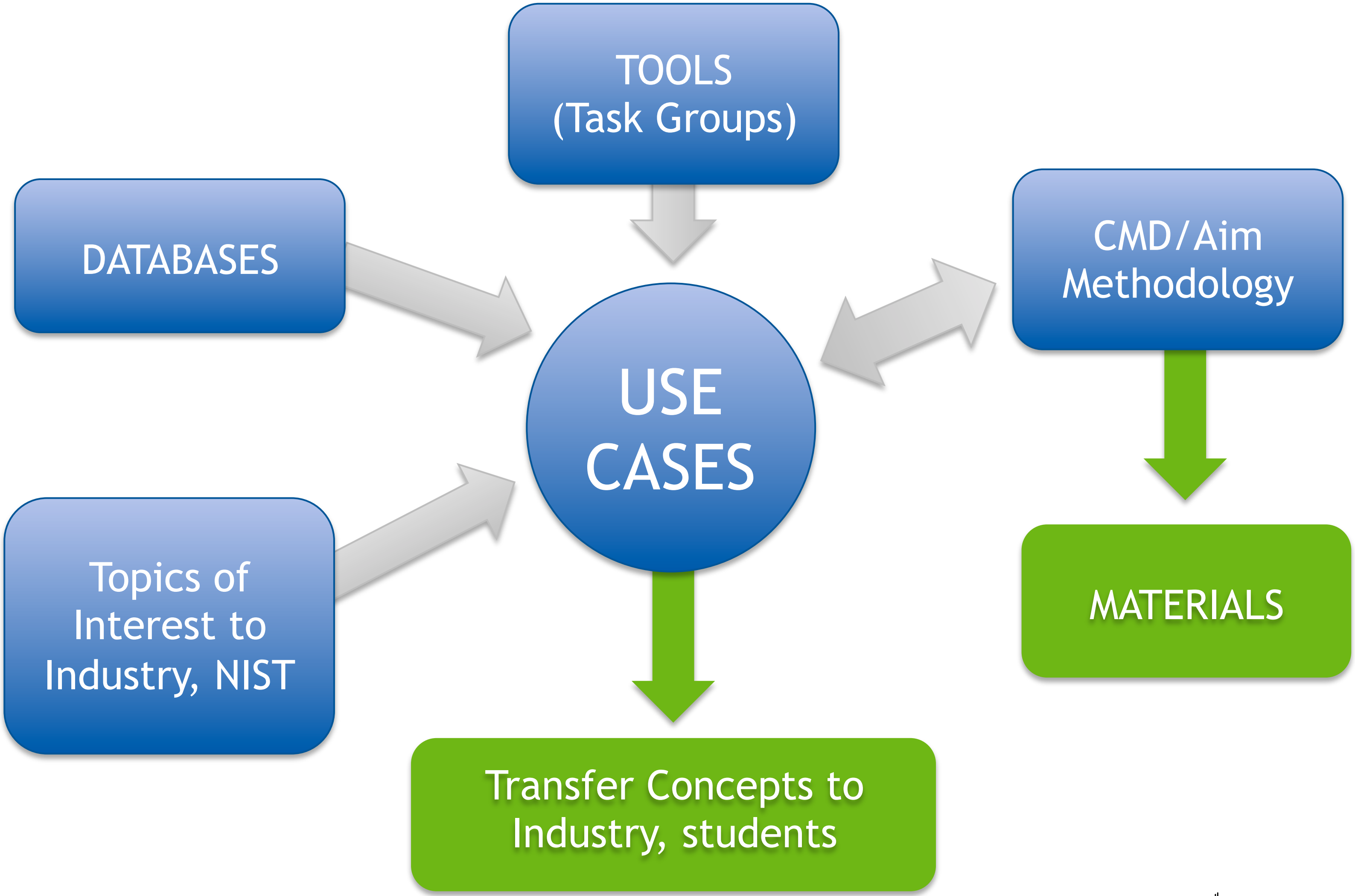
Mechanistic Models: Process-Structure and Structure-Property Models
Tools: *iCMD Platform*, *PrecipiCalc®*, Thermo-Calc, DICTRA, ABAQUS, DEFORM, D3D

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



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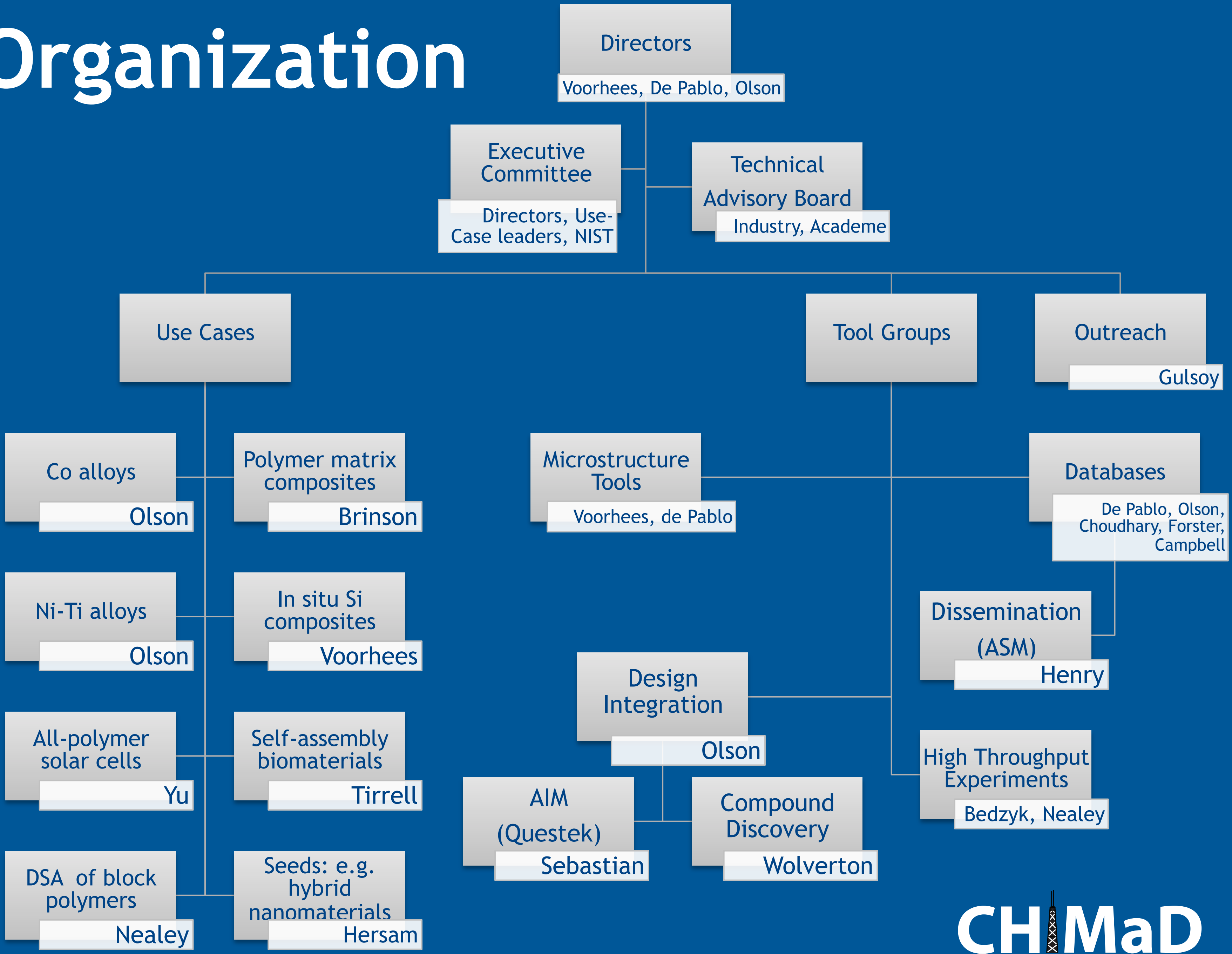
Organization



- Directors — Voorhees, De Pablo, Olson
  - Executive Committee — Directors, Use-Case leaders, NIST
  - Technical Advisory Board — Industry, Academe
  - Use Cases
    - Co alloys — Olson
    - Polymer matrix composites — Brinson
    - Ni-Ti alloys — Olson
    - In situ Si composites — Voorhees
    - All-polymer solar cells — Yu
    - Self-assembly biomaterials — Tirrell
    - DSA of block polymers — Nealey
    - Seeds: e.g. hybrid nanomaterials — Hersam
  - Tool Groups
    - Microstructure Tools — Voorhees, de Pablo
    - Databases — De Pablo, Olson, Choudhary, Forster, Campbell
      - Dissemination (ASM) — Henry
    - Design Integration — Olson
      - AIM (Questek) — Sebastian
      - Compound Discovery — Wolverton
    - High Throughput Experiments — Bedzyk, Nealey
  - Outreach — Gulsoy

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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 University, University of Chicago, and Argonne National Laboratory
- Summer schools
- Yearly TAB meetings

Tools

- Microstructure development
- Theoretically Informed Coarse Graining and Evolutionary Design
- Rapid Throughput and High Resolution Characterization
- Integration – Accelerated Insertion of Materials

Tools: 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

Cobalt Alloy Design

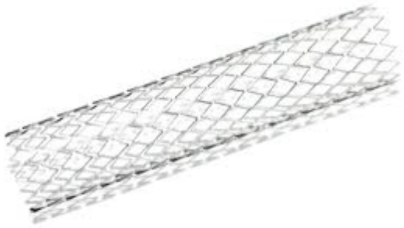
G. Olson (NU), D. Dunand (NU), D. Seidman (NU), P. Voorhees (NU),
M. Stan (NAISE, ANL), C. Wolverton (NU)

- 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

Nanodispersion-strengthened Shape Memory Alloys

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

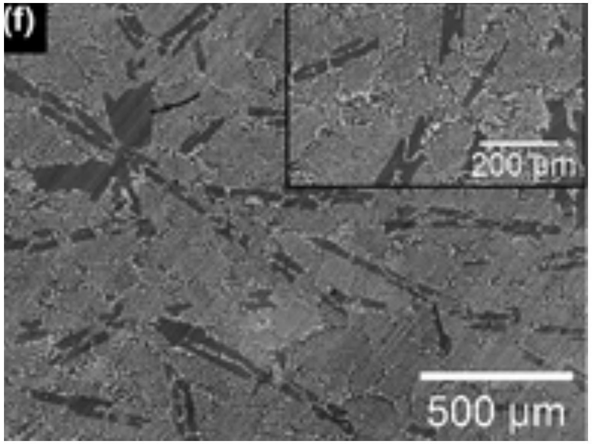
- Motivation:
  - Widely used in medical, aerospace and automotive sectors
  - Current alloys are susceptible to instability after many cycles
- Goals:
  - Near-term: Pd-stabilized alloys for medical devices
  - Long-term: High-temperature aeroturbine superalloy



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 in-situ 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. De Pablo (UC), H. Jaeger (UC),
M. Olvera de la Cruz (NU), S. Sibener (UC), L. Yu (UC)

Motivation

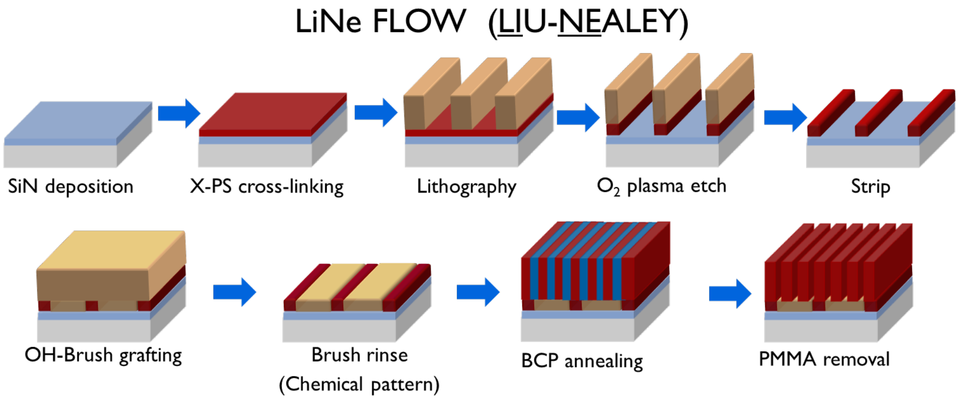
Lithography

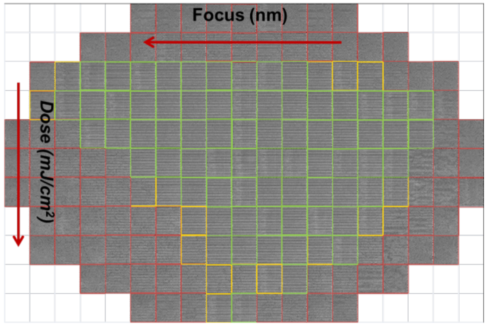
- Workhorse of semiconductor industry
- Important fraction of cost of electronic devices
- Need for new materials and processes for next-generation lithography
- Sub-10 nm patterning
- Need for metrology
- Need for design tool

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

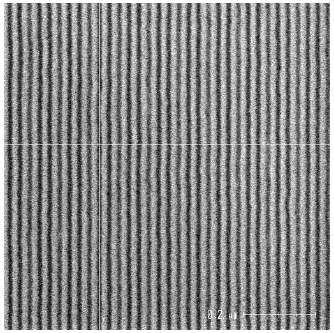




300 nm wafers

Track processing

IMEC



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Polymer Matrix Composites

C. Brinson (NU), J. De Pablo (UC), E. Luijten (NU),
J. Cao (NU), S. Keten (NU)

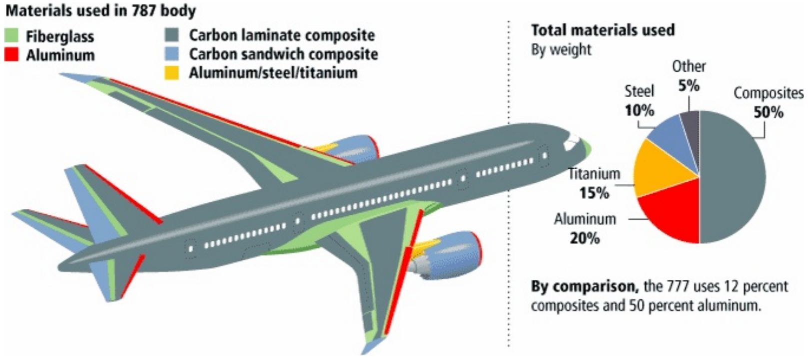
Motivation

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



By comparison, the 777 uses 12 percent composites and 50 percent aluminum.

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

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

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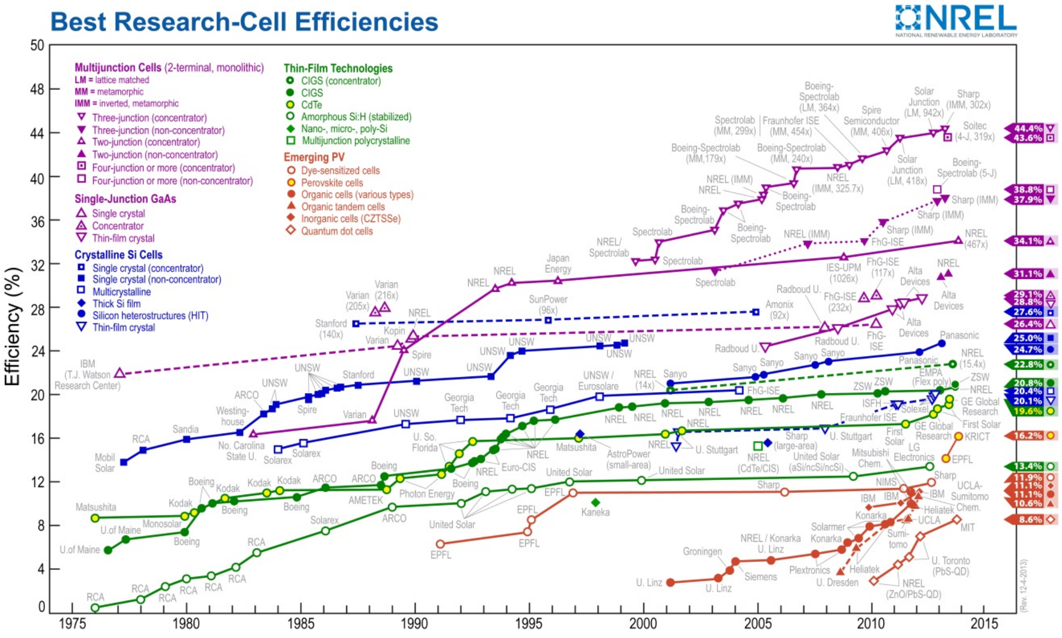
All-Polymer Organic Solar Cells

L. Yu (UC), 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 with high mobility for organic electronics

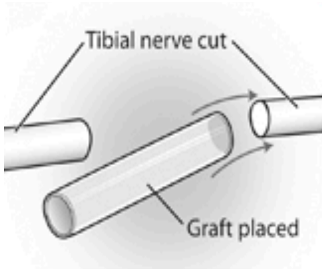
Self-Assembly of Biomaterials

M. Tirrell (UC), 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



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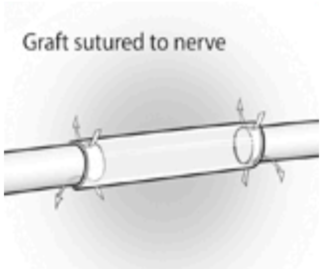

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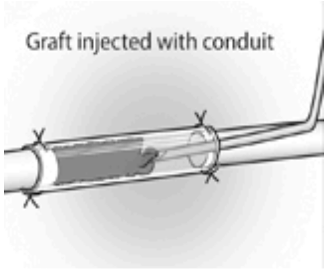

Seed Groups

Solution Processed Nanomaterials and Heterostructures
M. Hersam (NU), T. Marks (NU), L. Yu (UC), G. Galli (UC)

Non-planar Heterostructures
L. Lauhon (NU)

Deformation Processing
J. Cao (NU)

Expectations from Co-PI's

- Integration and collaboration is essential to the success of a use-case or tool group
- There will be a yearly review of the group's progress
- Decisions about seed groups will be made in year 3
- Research highlights should be submitted when papers are published