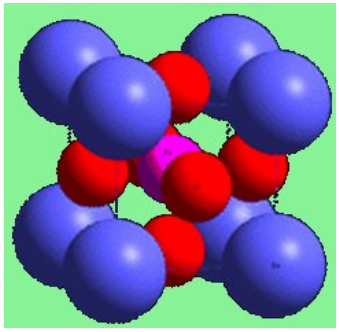
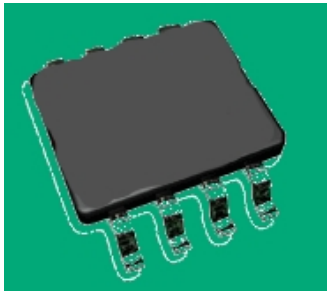
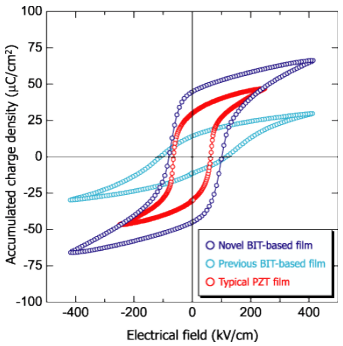
MATERIALS SCIENCE IN A NUTSHELL

Materials Science & Engineering

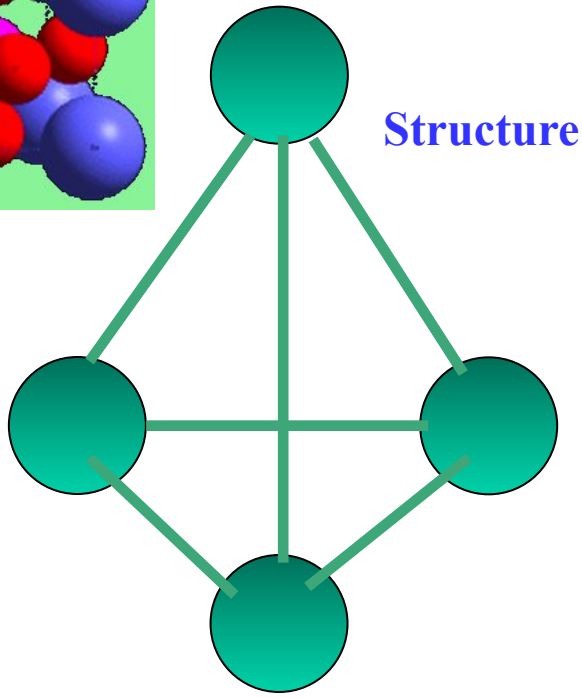


Structure



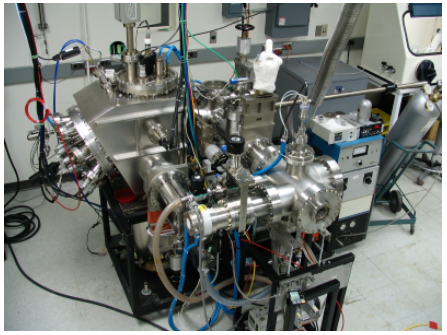


Property



Performance

Processing



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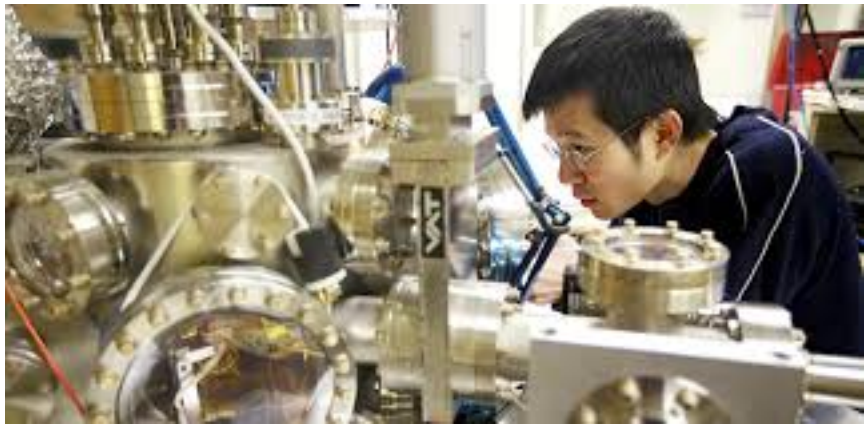

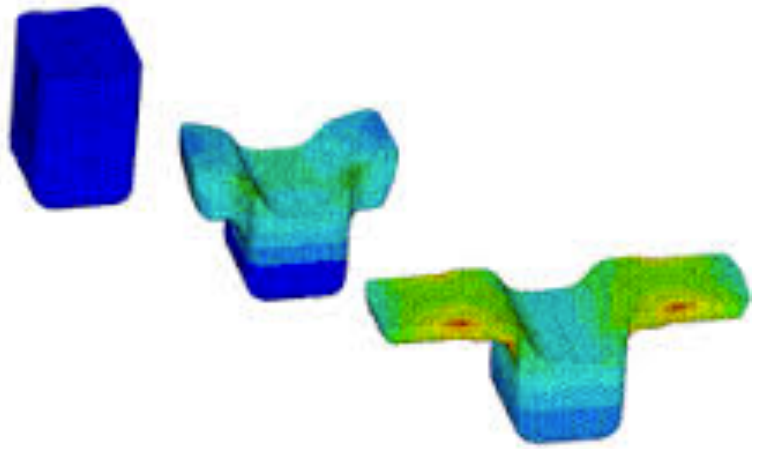

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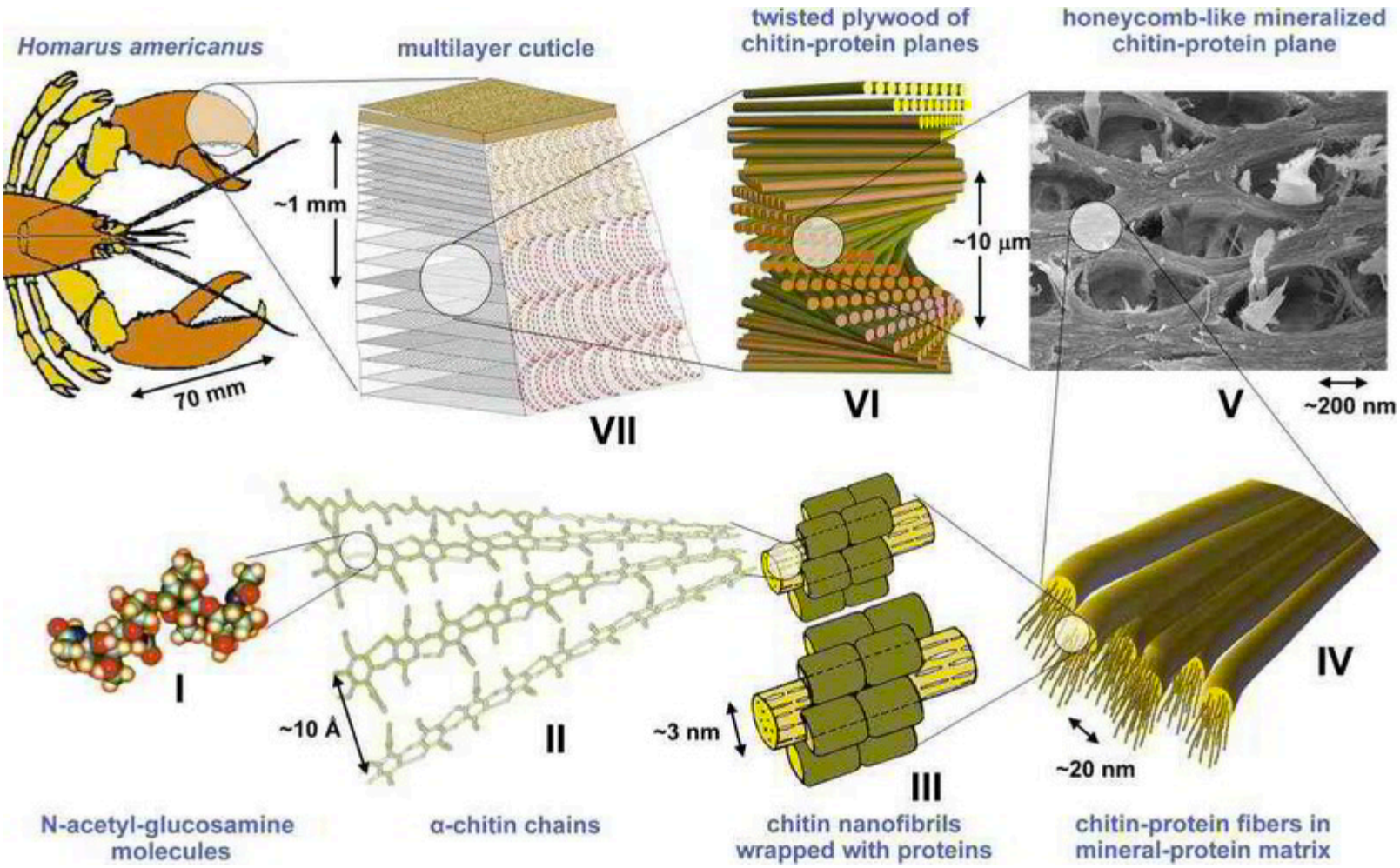
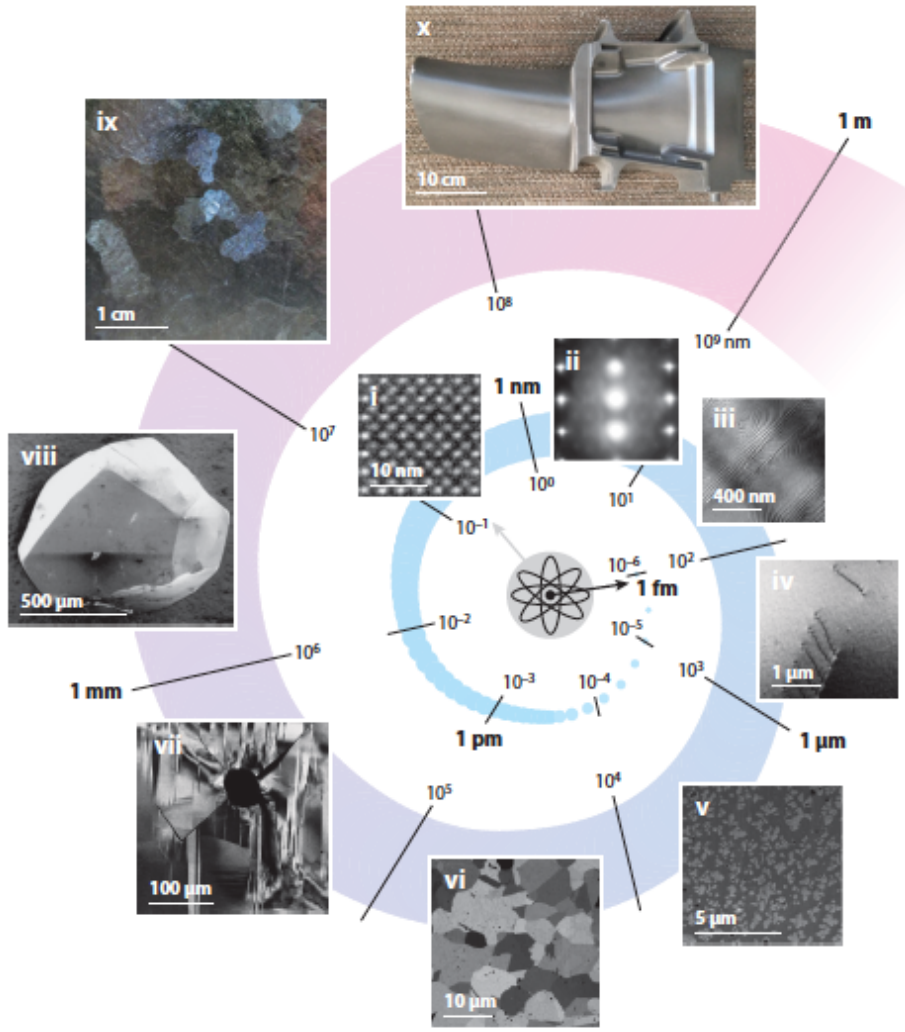


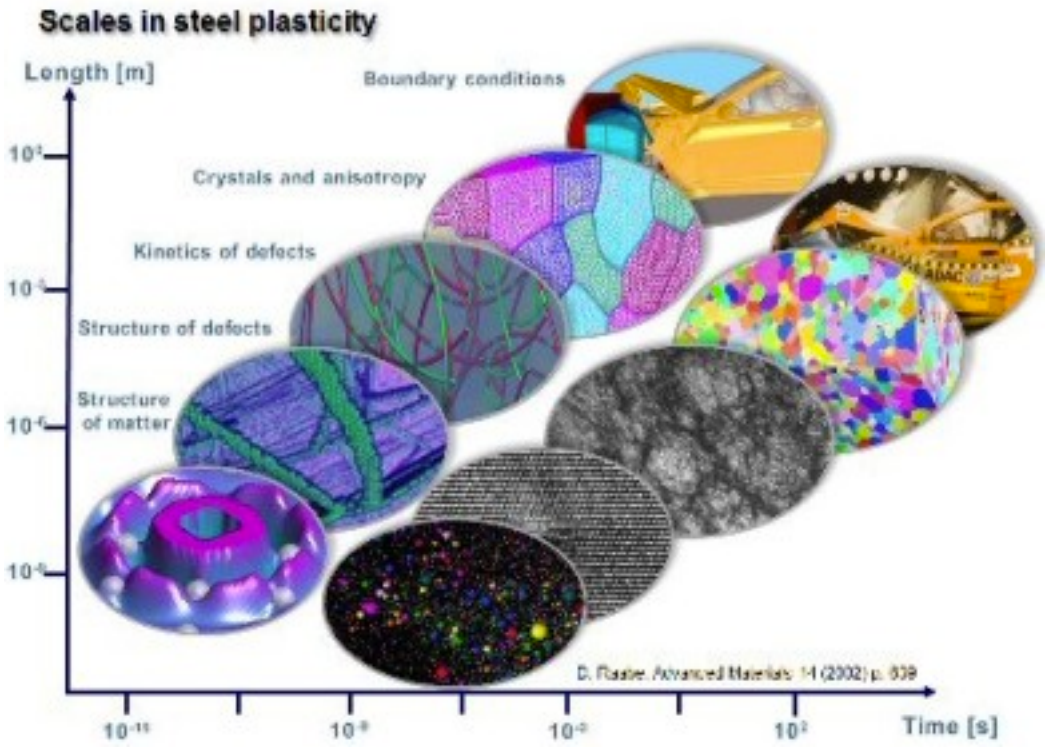
http://www.dierk-raabe.com/biological-natural-materials/chitin/

Structure



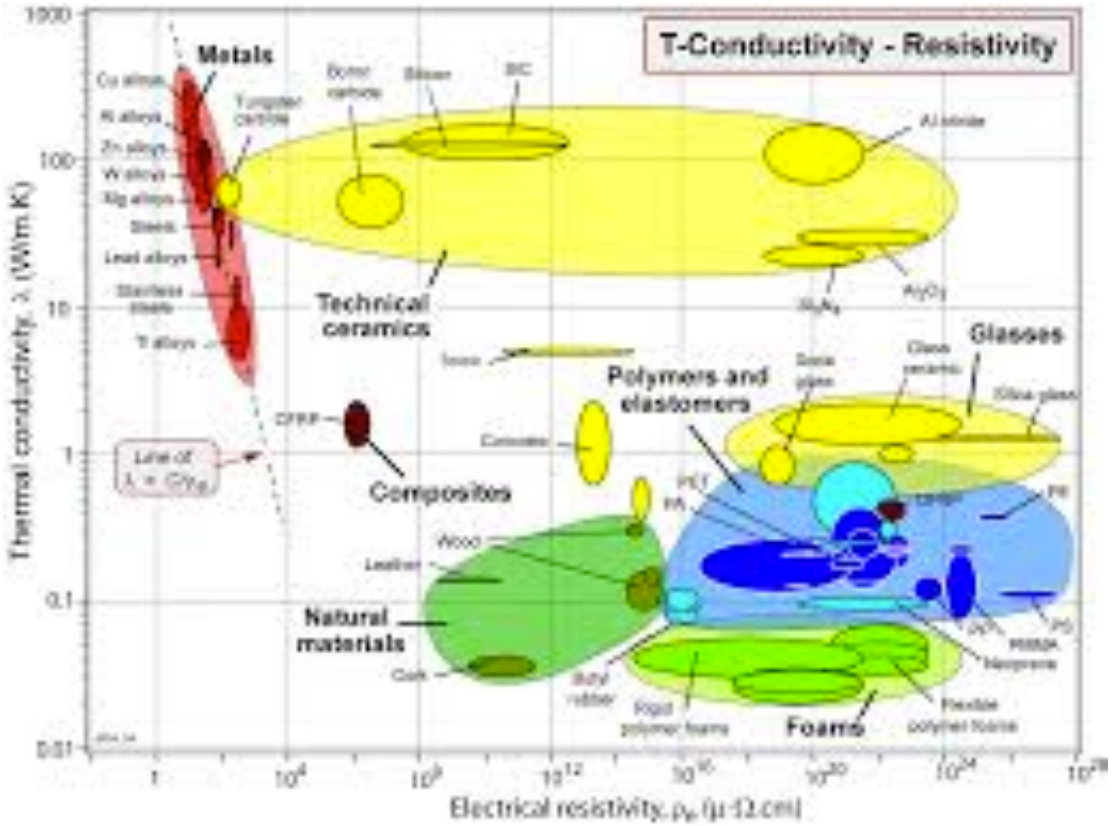
Annu. Rev. Mater. Res. 2015. 45:171–93

Multi-scale Nature of Materials

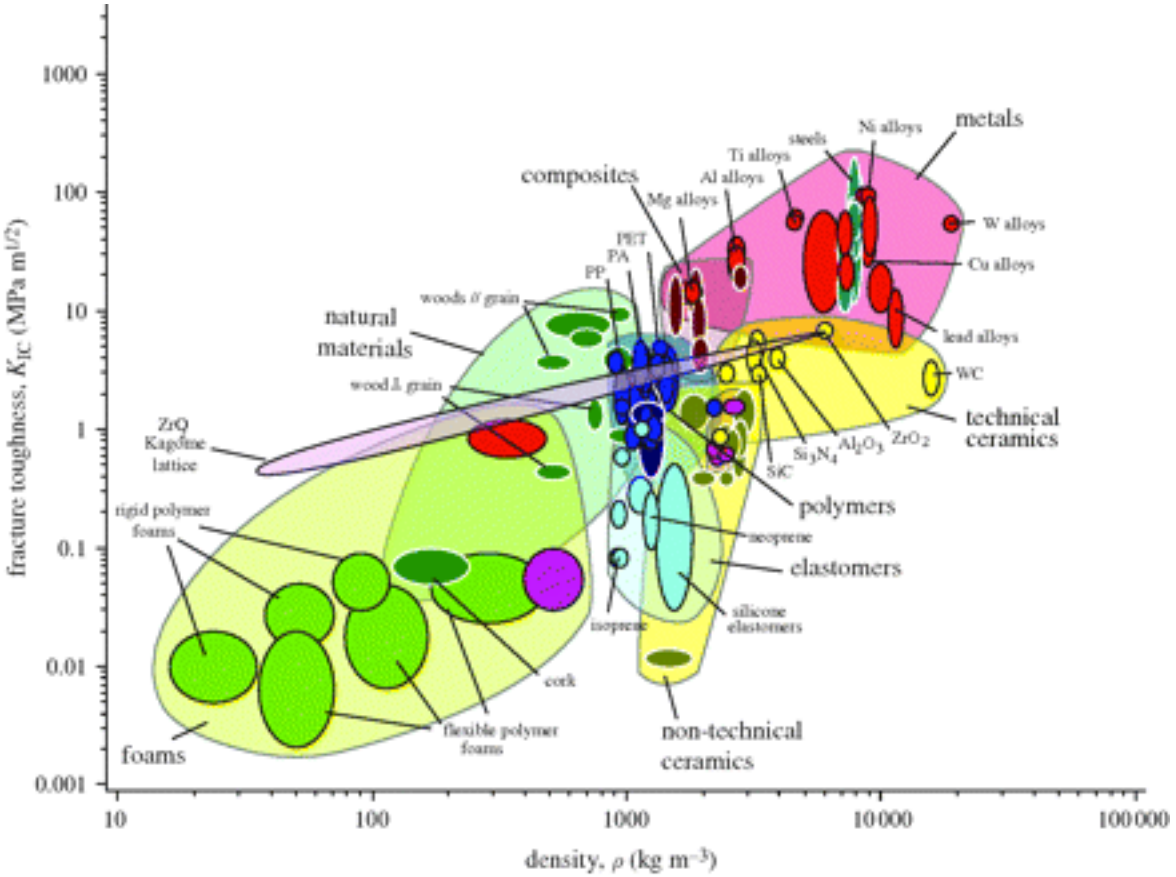


http://www.dierk-raabe.com/steel-properties-and-overview-images/

Properties

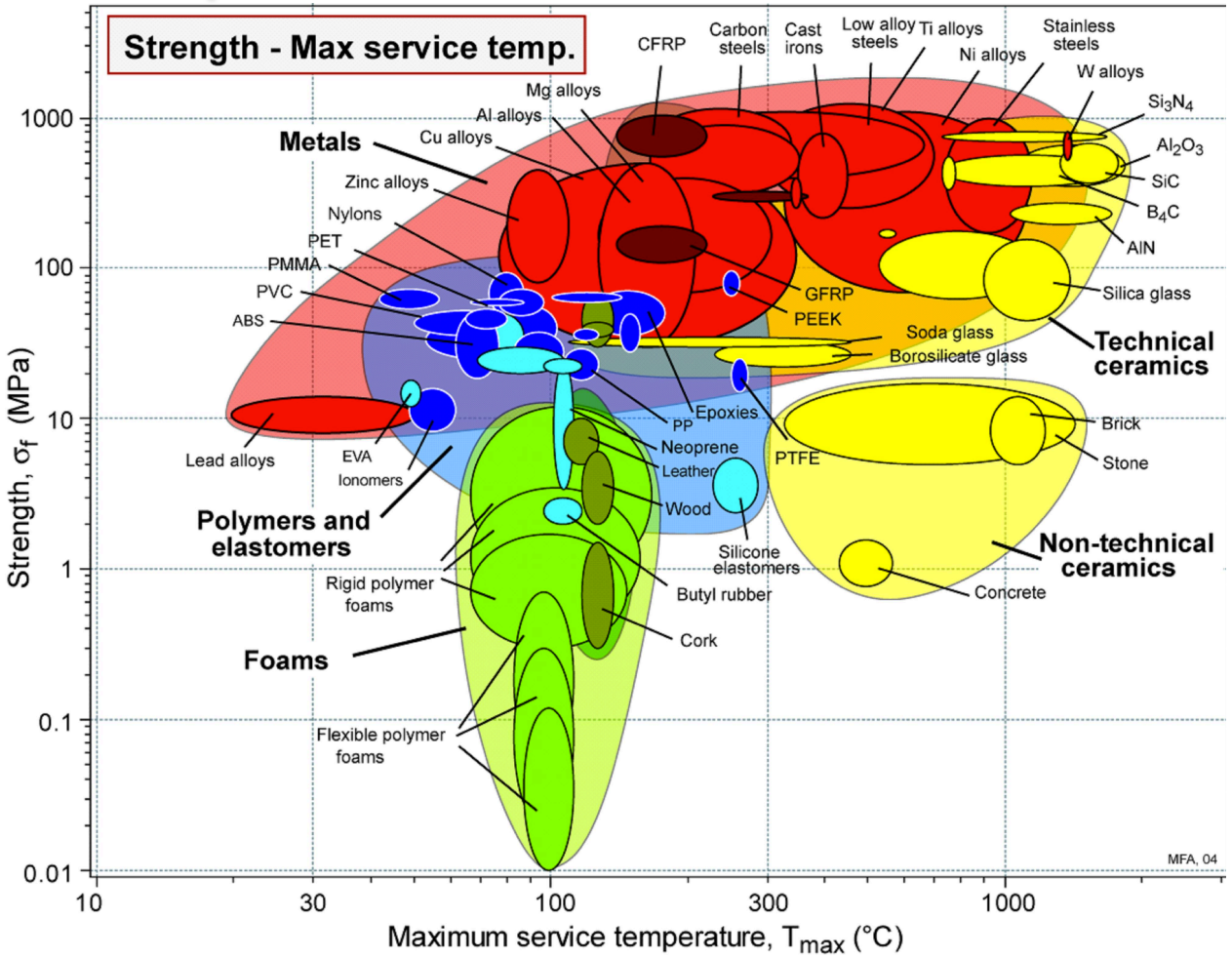

T-Conductivity - Resistivity
Metals
Technical ceramics
Glasses
Polymers and elastomers
Composites
Natural materials
Foams
Thermal conductivity, λ (W/m.K)
Electrical resistivity, ρe (μ Ω.cm)

Properties/Performance



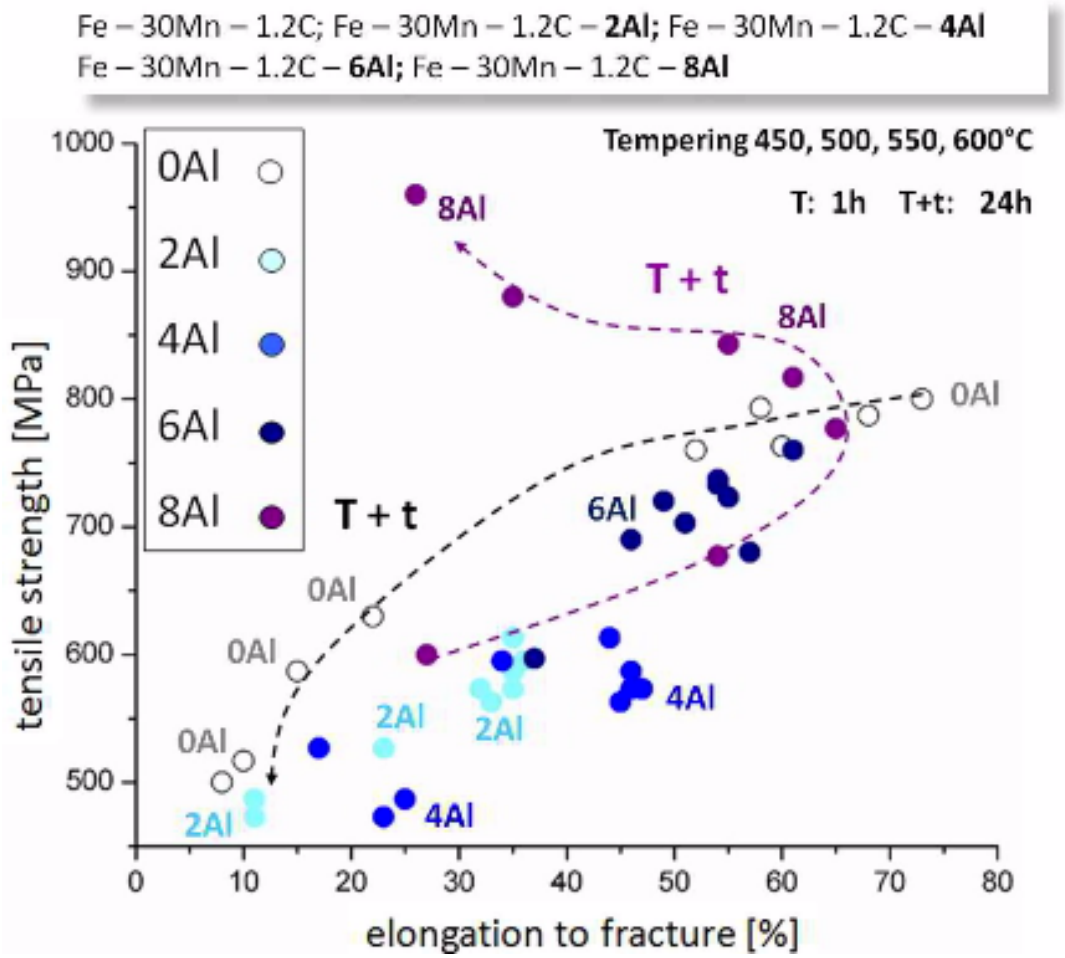
http://rspa.royalsocietypublishing.org/content/466/2121/2495

Properties/Performance



http://www.tangram.co.uk/TI-Polymer-High_temperature_plastics.html

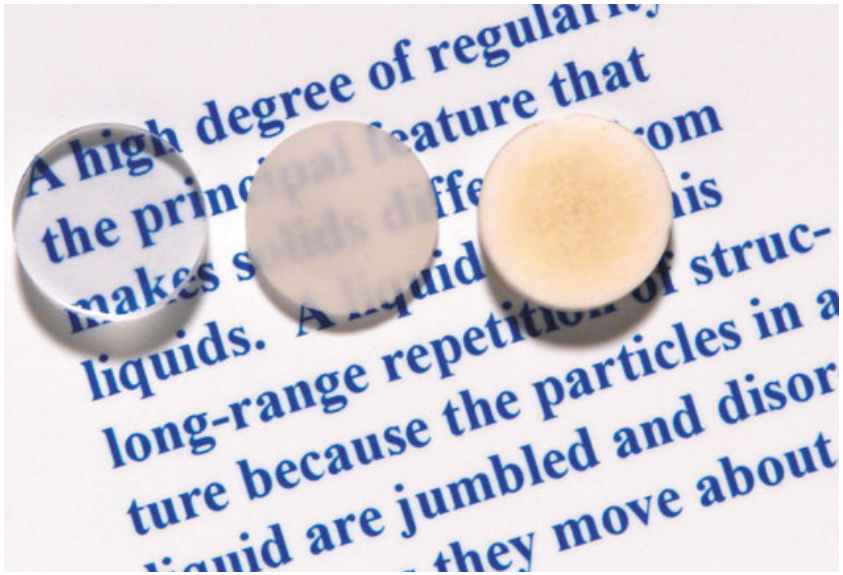
Properties



http://www.dierk-raabe.com/steel-properties-and-overview-images/

Structure ↔ Property

- Optical Properties of Al_2O_3
- All disks have same overall composition
- They have different structural characteristics



Material classification

- Metals
  - electron cloud
  - conductors
  - not transparent
  - strong
  - deformable
- Ceramics
  - insulators
  - high temperature resistance
  - resistant to harsh environments
  - hard
  - brittle

Material classification

- Polymers
  - organic
  - large molecular structures
  - flexible
- Composites
  - combined properties
- Semiconductors
  - sensitive to impurities
- Biomaterials
  - implants
  - compatible, nontoxic

Material Properties

- Categories
  - mechanical
  - electrical
  - thermal
  - optical
  - magnetic
  - deteriorative / chemical
- Characteristic stimulus
  - load / stress
  - electric field
  - temperature gradient
  - light radiation
  - magnetic field
  - dimensional requirement
  - environment

- connect “causes” (stimulus) & “responses”

Material Properties

- mechanical
  - stiffness
  - strength
  - ductility
  - toughness
- electrical
  - conductivity
  - dielectric constant
- thermal
  - heat capacity
  - conductivity
  - coeff of expansion / contraction
- optical
  - index of refraction
  - reflectivity
- magnetic
  - permeability
- deteriorative
  - chemical reactivity

Properties of matter depend on

- chemical bonding (scale = <1A)

which depends on quantum mechanics and electrodynamics;

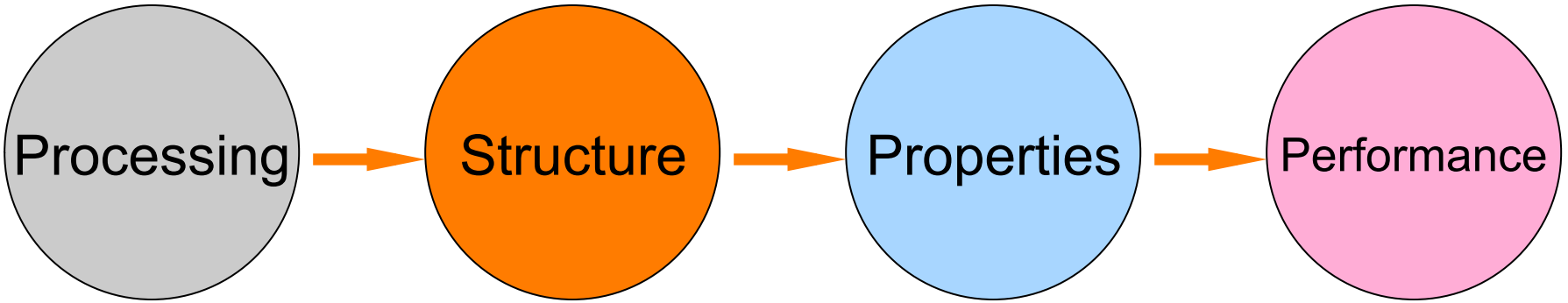
- crystal structure (scale ~ 1-10A)

which depends on chemical bonding and statistical mechanics;

- microstructure (scale ~10^2-10^6A)

which depends on bonding and statistical mechanics, collective effects);

The key components of materials science and engineering



- materials science - investigate relationships
- materials engineering - using relationships to engineer structure to produce required properties

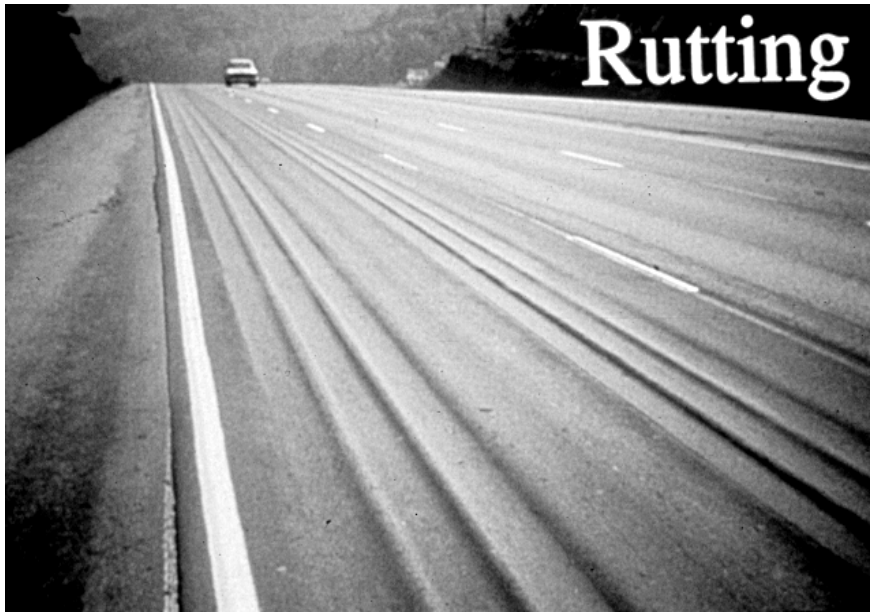
Material Selection

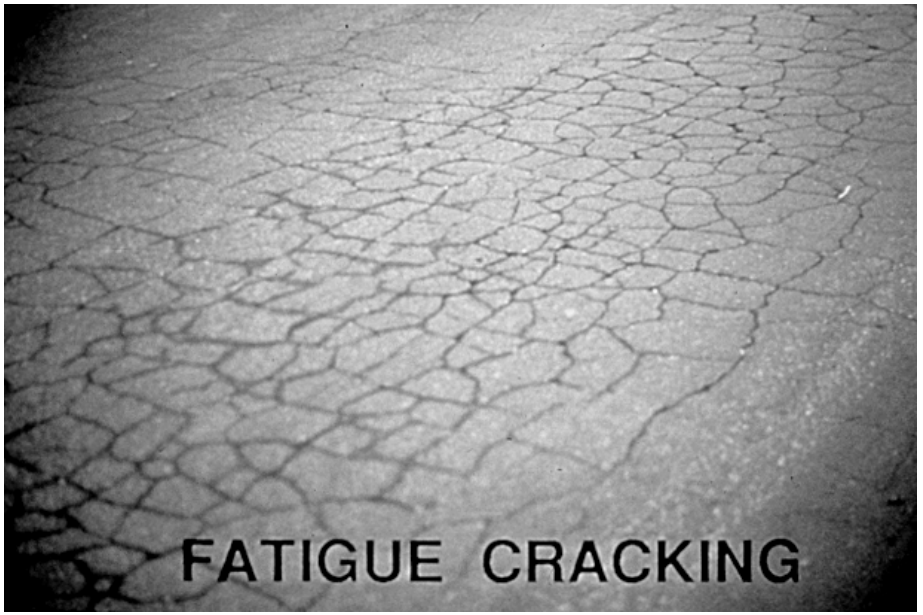
- **Team Activity**

Give an example (application or product) where at least three of the following types of properties has to be considered when choosing the materials

- mechanical
- electrical
- thermal
- optical
- magnetic
- biocompatible
- chemical or corrosion resistance

Balancing Properties



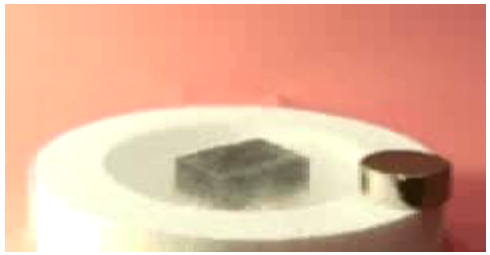


Too compliant: it deforms

Too stiff: it cracks

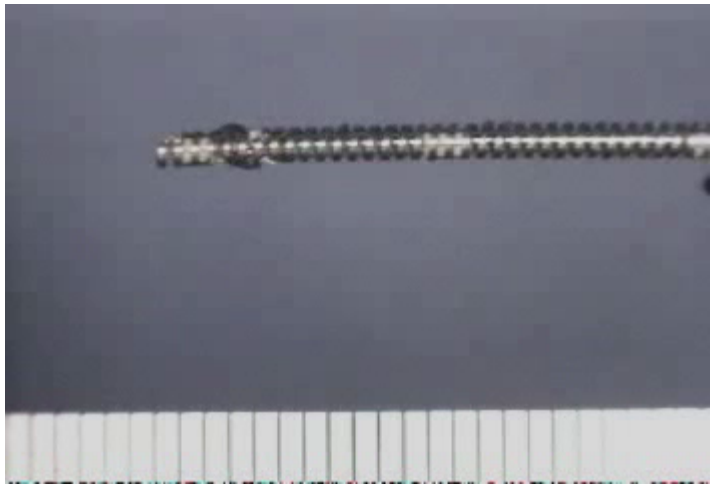
Technological breakthroughs enabled by development of materials

- Micro-electronics:
  - Discovery of semiconducting properties of Silicon and Germanium (~1940s)
- Nuclear-Magnetic Resonance Devices:
  - Superconducting Nb-based coils (superconductivity in metals discovered ~1905)
  - High temperature superconductors (?)
- Efficient Jet engines:
  - Development of precipitate strengthening super alloys (~1950s)



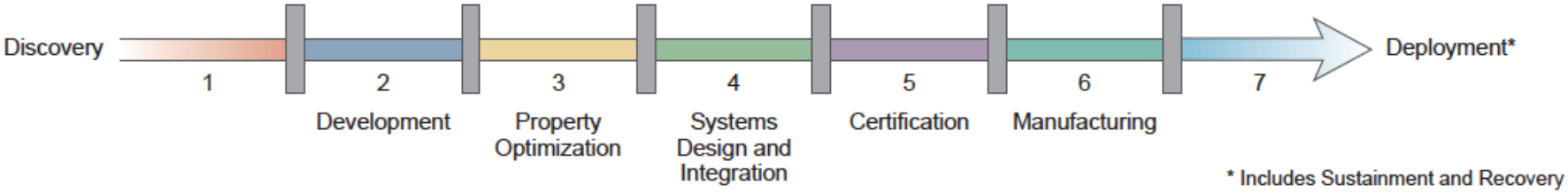
Technological breakthroughs enabled by development of materials-recently(!)

- Hydrogen-based economy:
  - Development of novel hydrogen storage materials (ongoing)
- Nanotechnology:
  - Nano-materials
    - Carbon Nano-tubes (~1990s)
    - Nano-wires (~2000)
    - Etc
- Active Materials
  - Shape Memory Alloys (~1990s)
  - Shape Memory Polymers (~1990s)
- Bio-engineering
  - Virus-grown nano-materials (~2000)
  - Bio-inspired materials (~1990s)



THE NEED TO ACCELERATE MATERIALS DEVELOPMENT

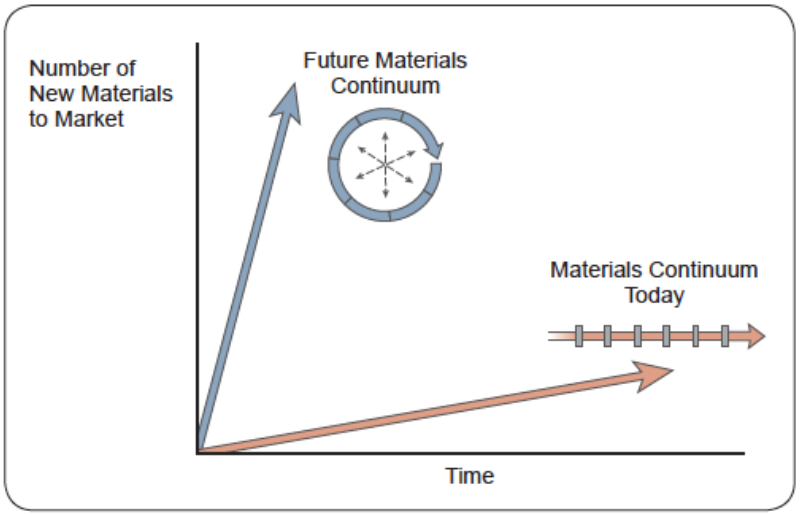
Materials Genome Initiative

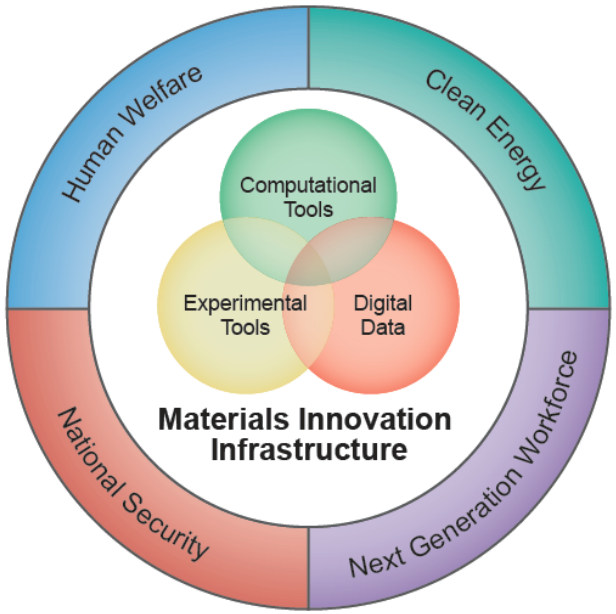


Typical Time Frame ~ 15- 20 years!!!

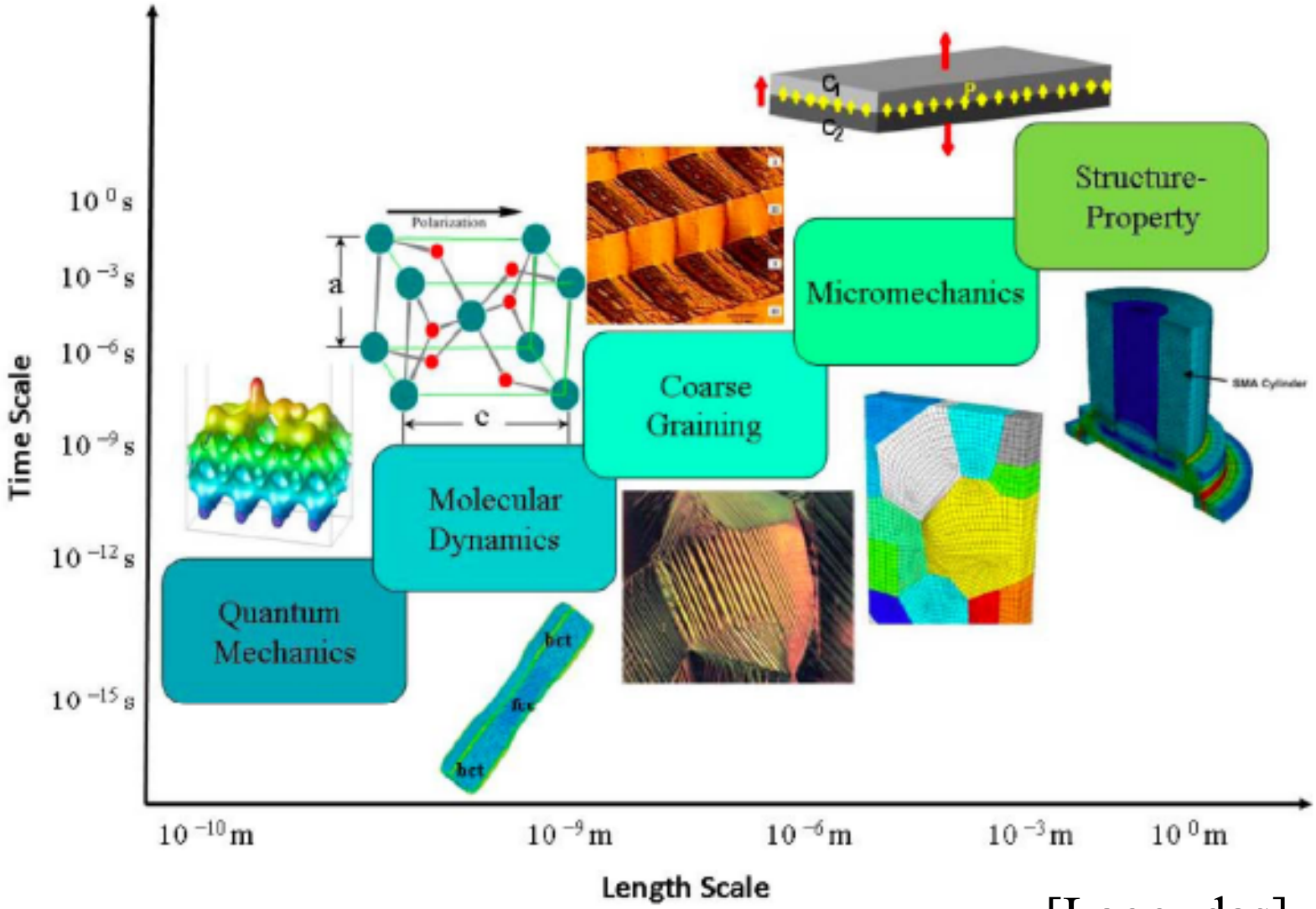
Current activities: The Materials Genome Initiative:

Goal: Reduce Cost and Time by Half



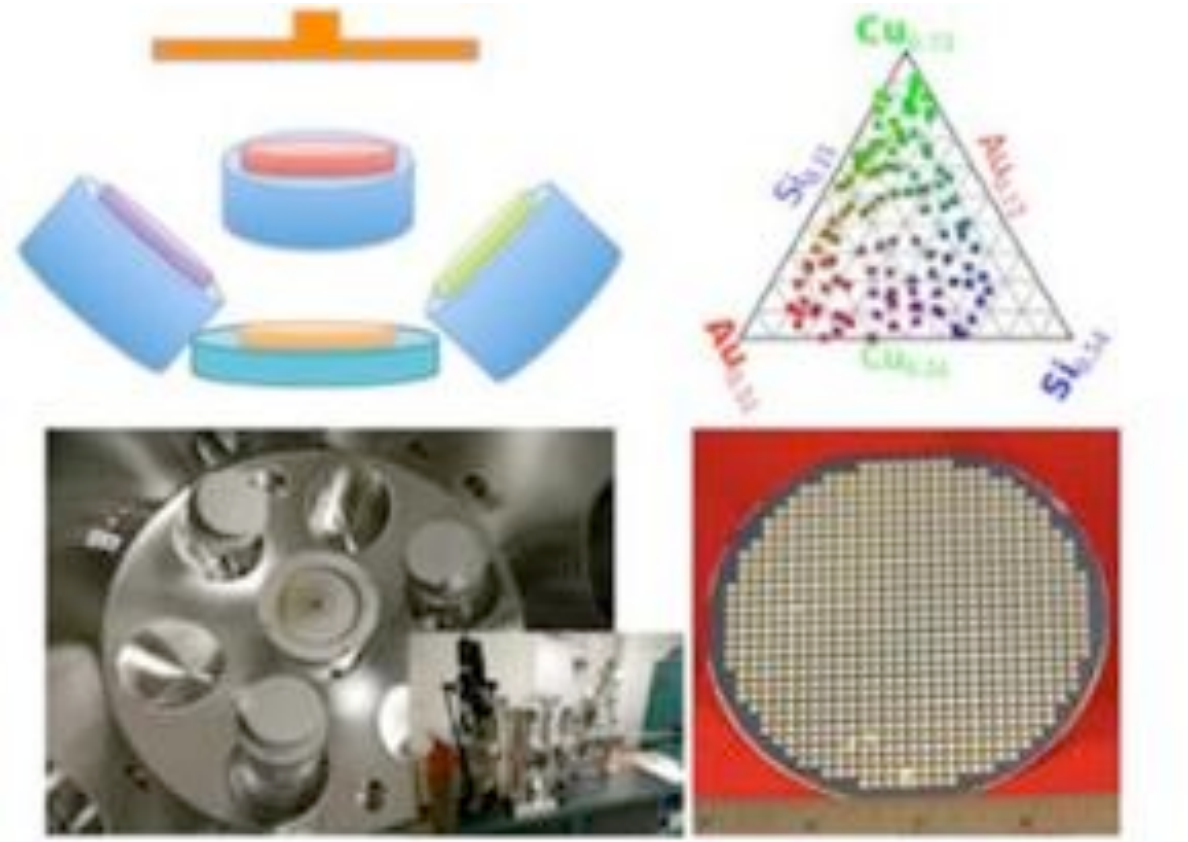


MGI: Multi-Scale Modeling



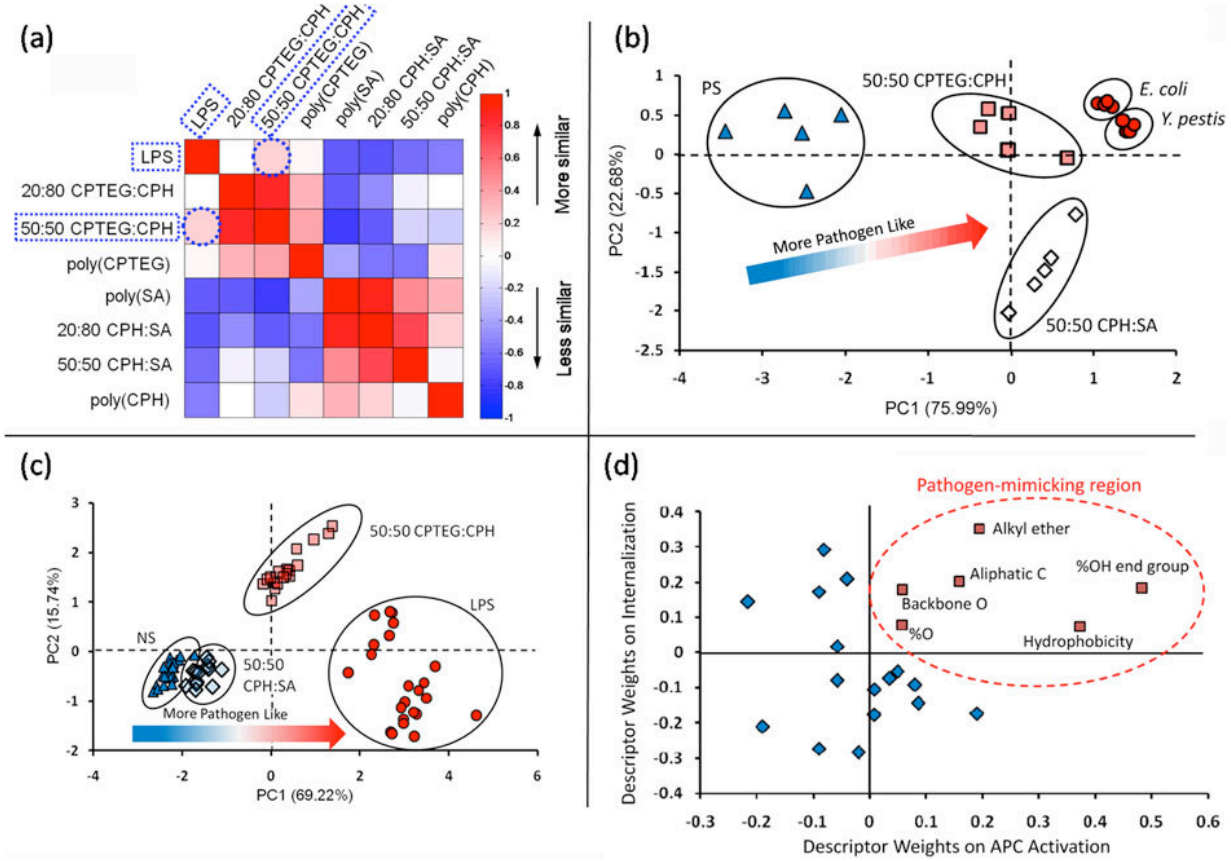
[Lagoudas]

MGI: High Throughput Synthesis/ Characterization



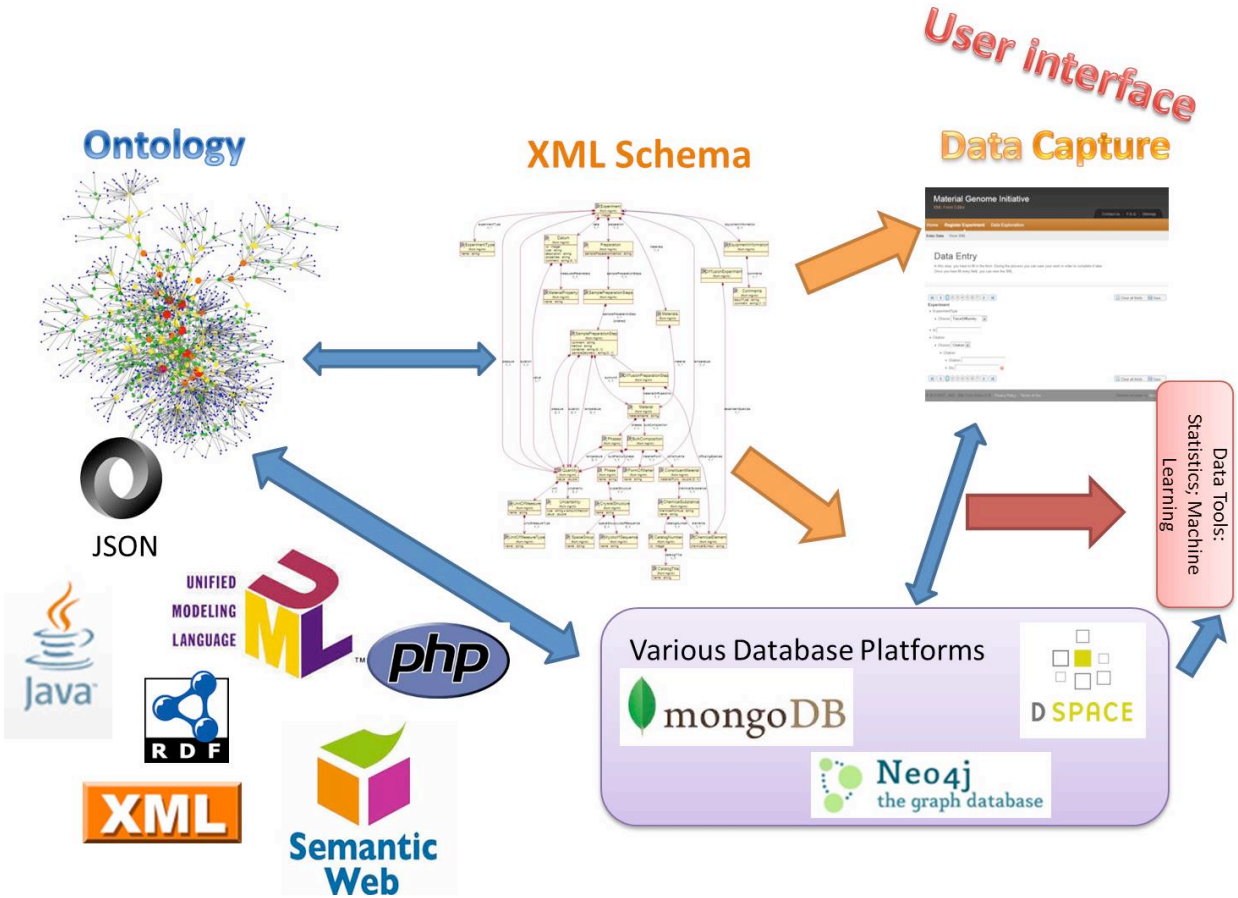
[UCLA MURI]

MGI: Materials Informatics



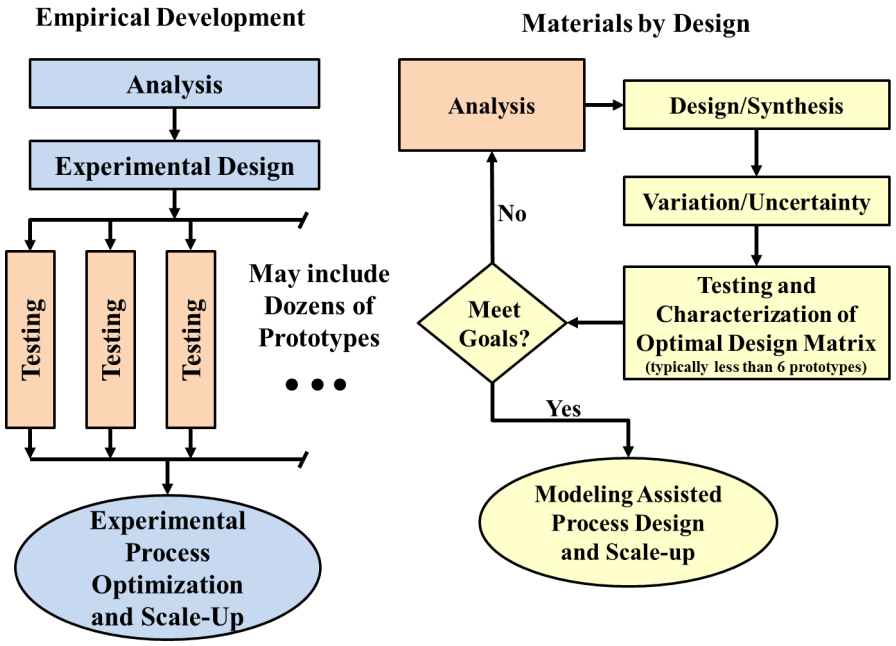
[Ulery et a, Nature 2011]

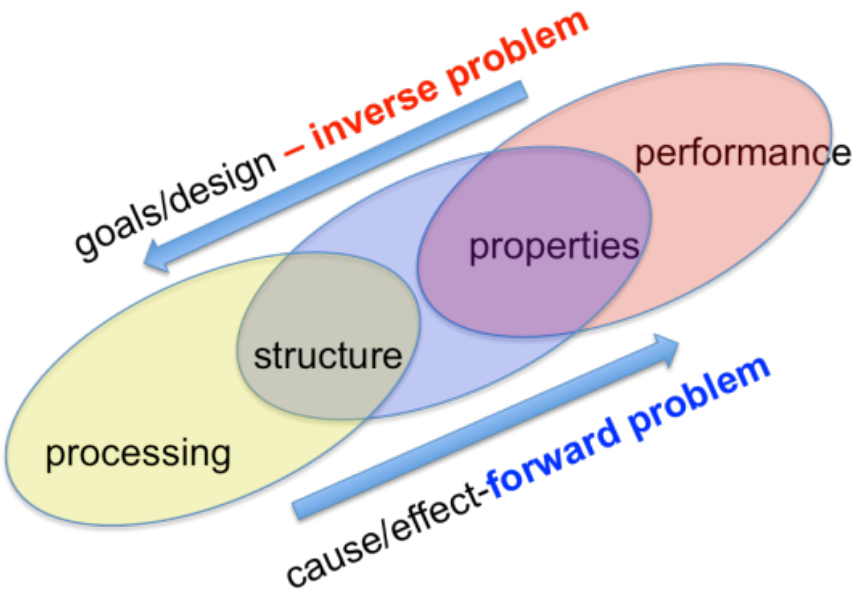
MGI: Information Infrastructure



[NIST, Materials Genomics Gr

MGI is about solving **forward** and **inverse** problem in MSEN

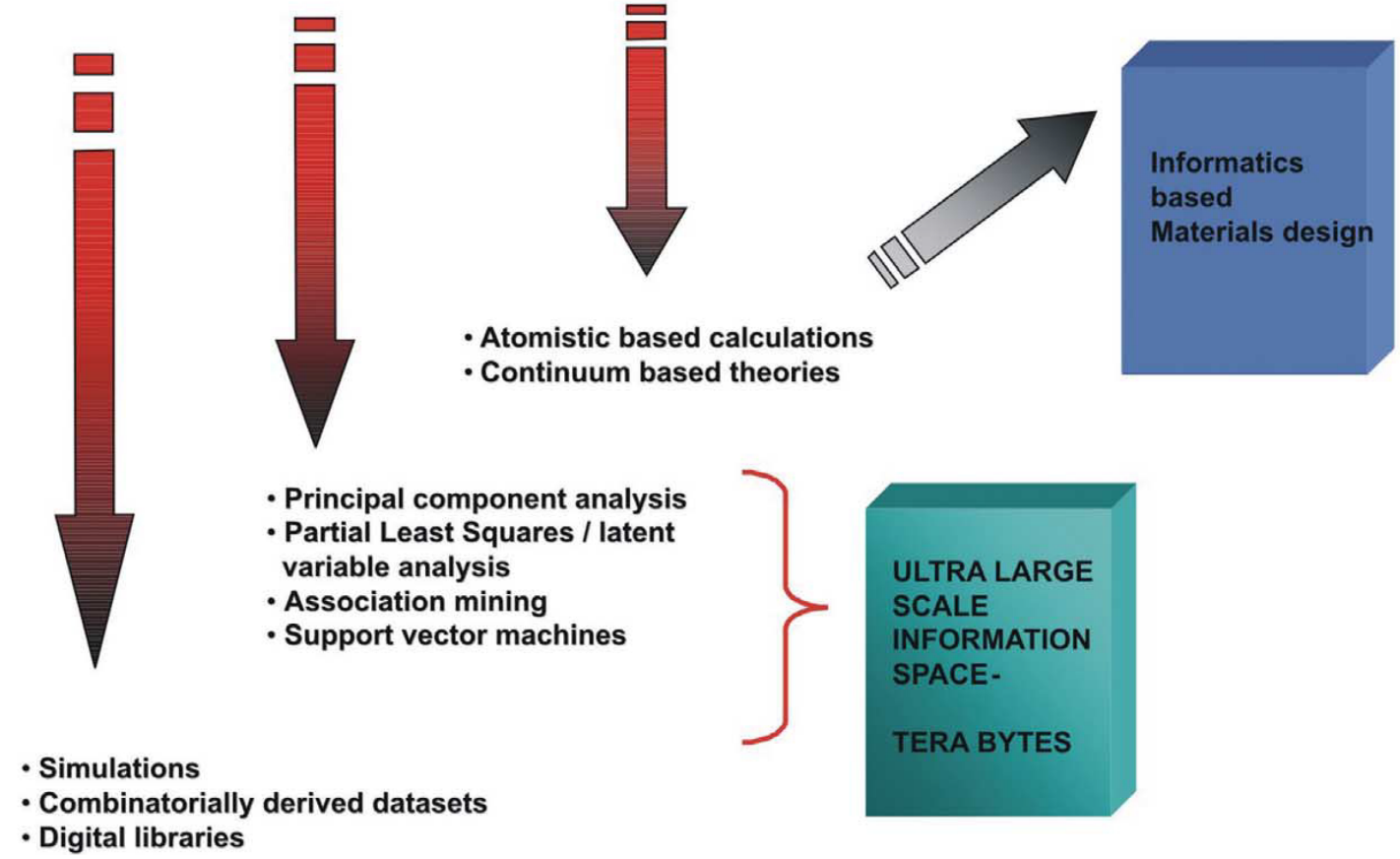




MATERIALS INFORMATICS

Getting Knowledge out of Data

Data + Correlations + Theory = Knowledge-base



2005 Rajan

Informatics

What is it ?

- Searching for patterns of behavior among multivariate data sets
- Can pattern recognition lead to predictions?

Why ?

- Establish new correlations
- Identify outliers
- Enlarge database / virtual libraries
- Evaluate databases
- Establish predictions

Informatics

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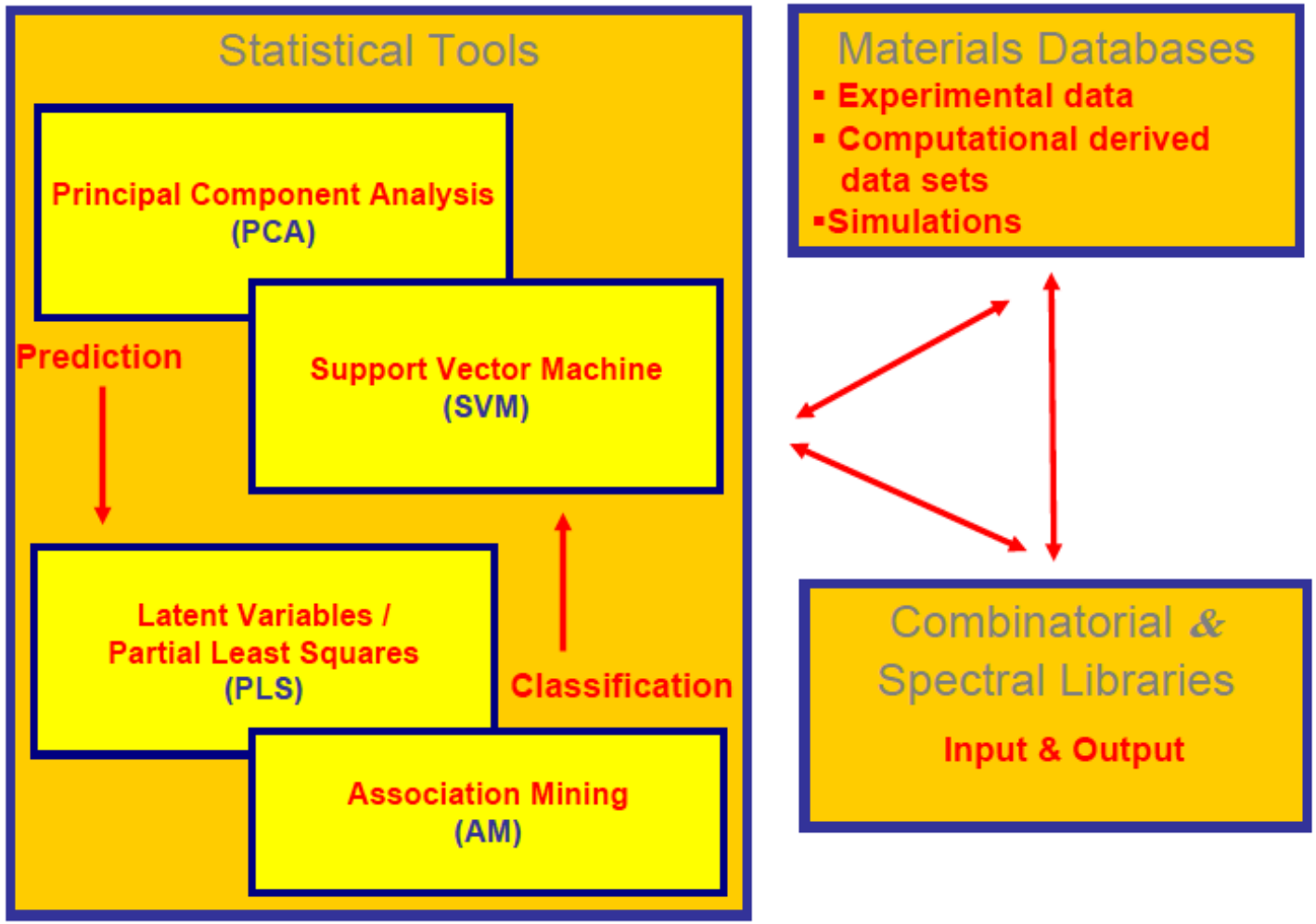
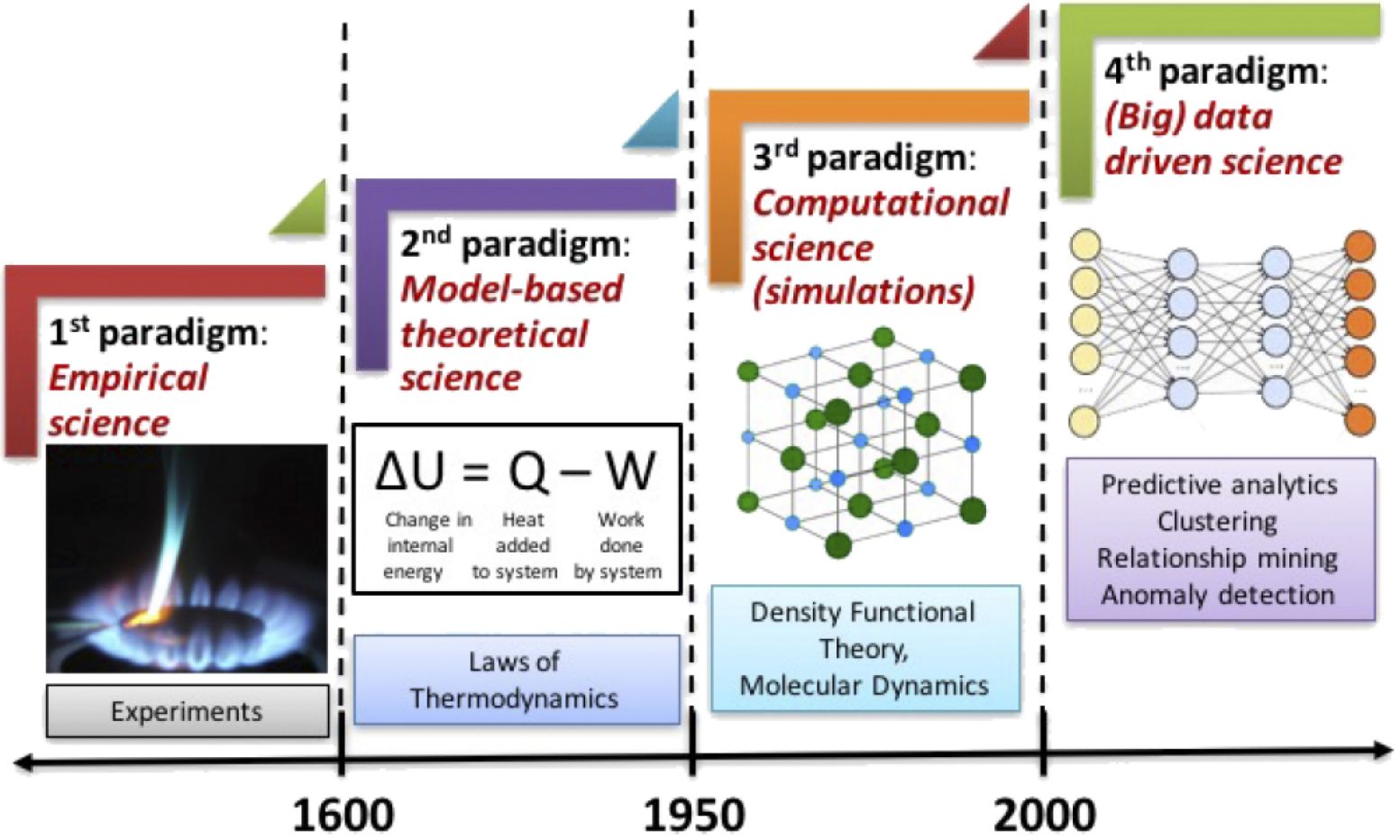
Materials Informatics

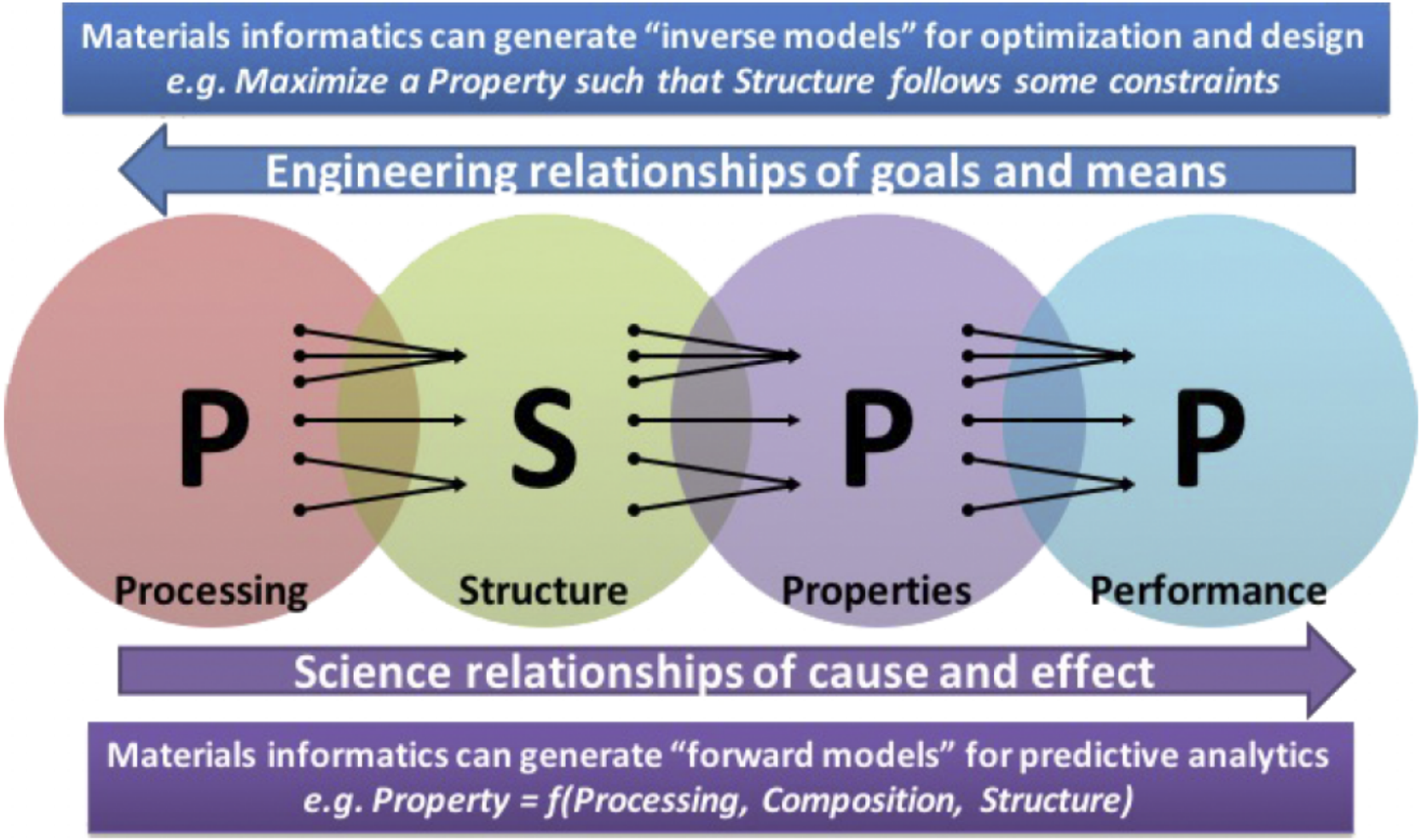


The Fourth Paradigm



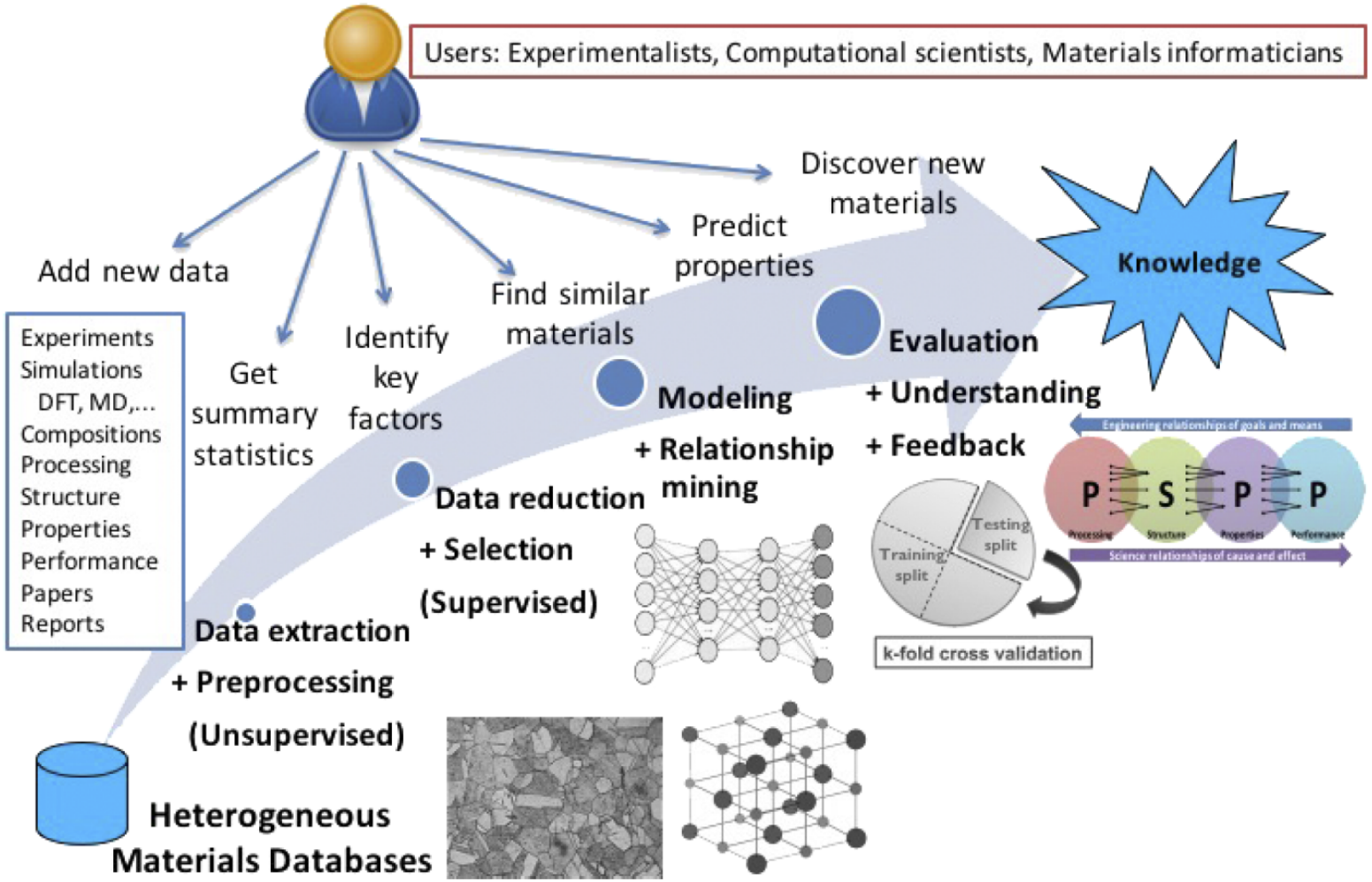
2016 Agrawal (APL)

QSPRs



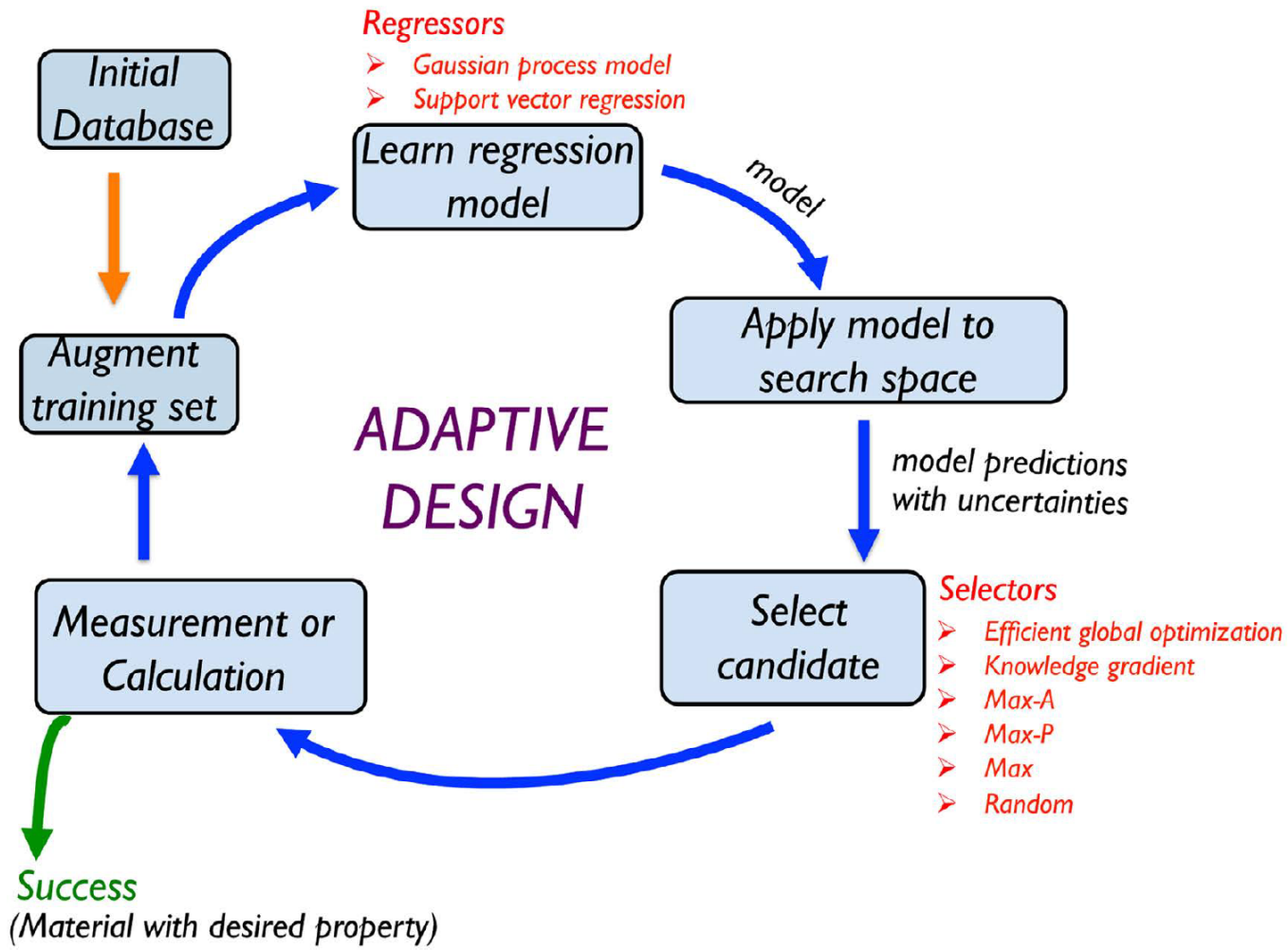
2016 Agrawal (APL)

Data-Enabled Materials Discovery Workflow



2016 Agrawal (APL)

MI as an Enabling Tool for Materials Development



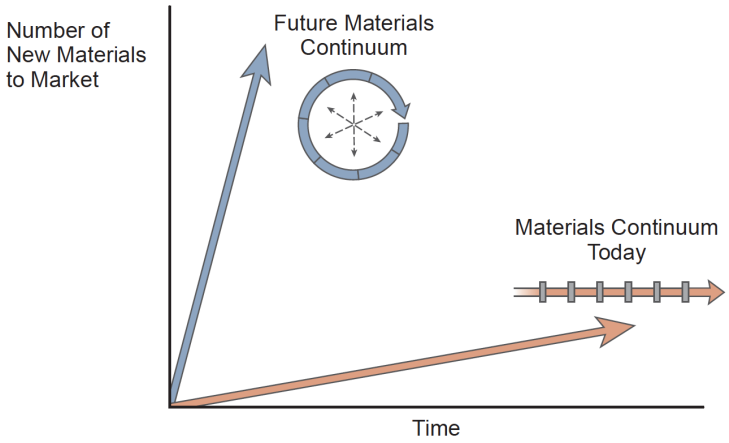
D3EM

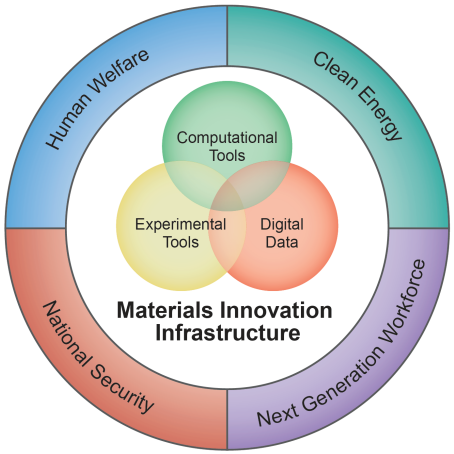
SHAMELESS ADVERTISEMENT

D^{3}EM: Data-Enabled Discovery and Design of Energy Materials- NSF-DGE-1545403

Materials Genome Initiative

Accelerating Materials Development by combining: Experiments, Models,





MGI's Three Pillars:

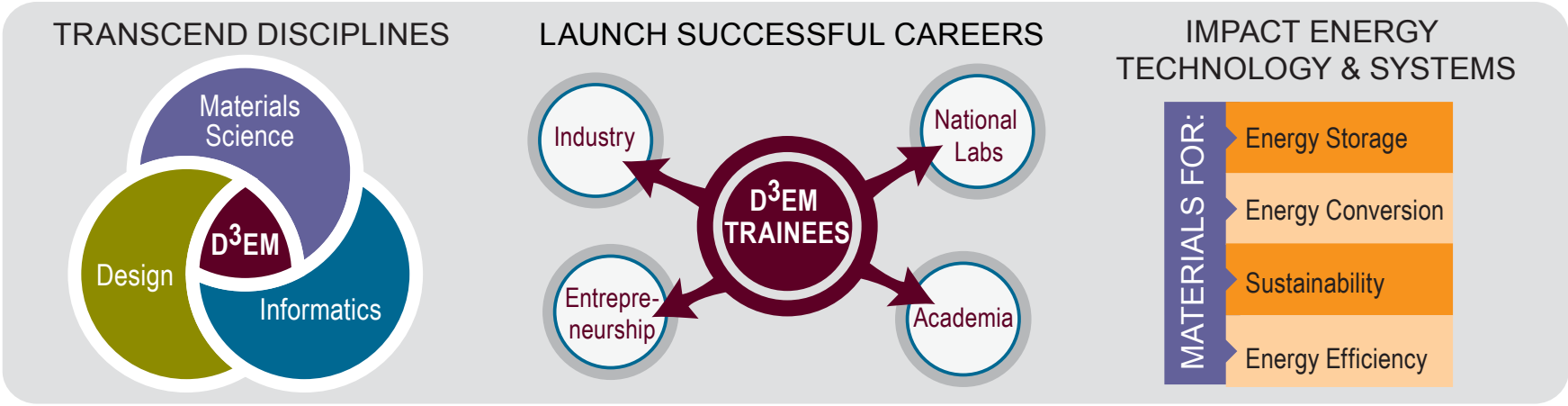
D^{3}EM's Contribution

- Developing a Materials Innovation Infrastructure
- Achieving National Goals With Advanced Materials
- Equip Next-generation Work Force

D^3EM: Data-Enabled Discovery and Design of Energy Materials

SIX DEPARTMENTS • THREE DISCIPLINES • ONE VISION

Building a collaborative framework for the accelerated development of materials through materials science, informatics, and engineering design.



PI: R. Arroyave, Co-PIs: D. Fowler, R. Malak, E. Dougherty, J. Ross
SP: M. Radovic, H. Zhou, J. Lutkenhaus, D. Allaire, S. Banerjee, P. Shamberger

College of Science: Chemistry, Physics

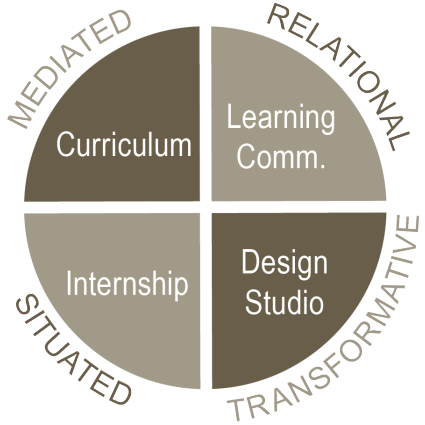
College of Engineering: Materials Science, Chemical Engineering, Mechanical Engineering, Electrical and Computer Engineering

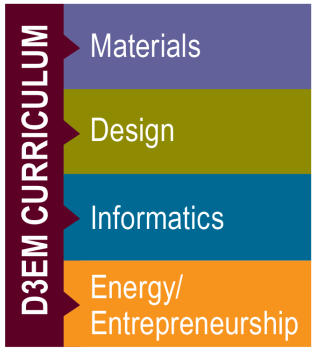
D^{3}EM: Data-Enabled Discovery and Design of Energy Materials

Integrating Education and Research

EDUCATION

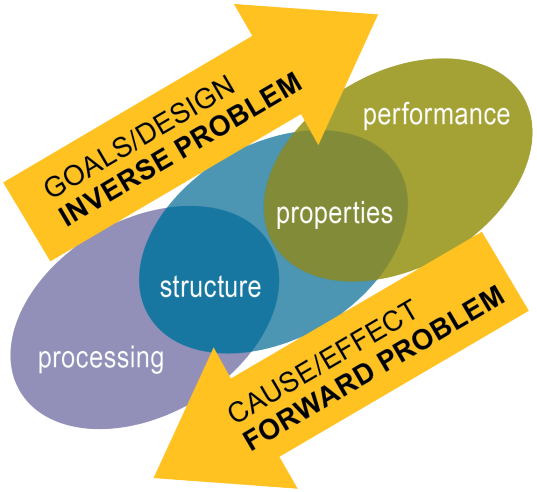
PEDAGOGICAL MODEL





Emphasis on Developing Employer-desired Professional and Technical Skills

RESEARCH



- Impact of Pedagogical Methods
- Goal Oriented Materials Design
- Data-Enabled Materials Discovery

Highly Interdisciplinary Training and Research Programs

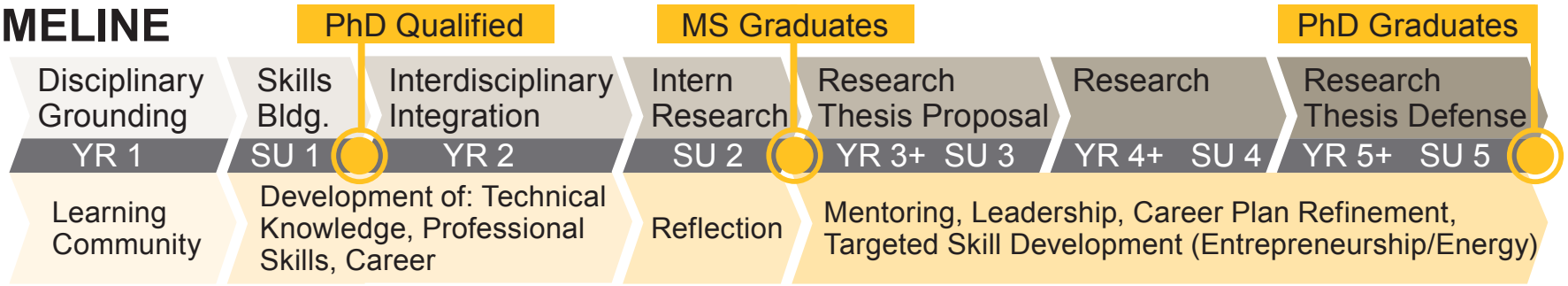
D^{3}EM: Data-Enabled Discovery and Design of Energy Materials

Main Features of D^{3}EM

KEY FEATURES:

- Employer-driven Learning Outcomes
  See survey results: Table 2, Page 6
- Disciplinary Grounding followed by Interdisciplinary Learning
- Reflection through e-Portfolio
- Learning Community
- Faculty Community of Scholars
- Summer School on Computational Materials Science
- Capstone Materials Design Studio
- Energy and Entrepreneurship
- Research on Pedagogical Impact and Dissemination in Scholarly Literature

TIMELINE



LEADERSHIP	**9** NRT Faculty • **10+** Affiliated • External Advisory Board • Internal Admin. Council
TRAINEES	**41** NRT-funded MS, PhD Students • **40+** Additional Participants • **2** Education PhDs
INCLUSION	Broad Recruitment Strategies • Partnership w/ URM Schools • Targeted Fellowships Learning Community • Faculty/Peer Mentoring • Individual Development Plan

http://d3em.tamu.edu

D^{3}EM: Data-Enabled Discovery and Design of Energy Materials

New Certificate Program

Competitive Fellowships Available!

Launching in 2016:

http://d3em.tamu.edu