Survey of Materials. Lecture 1

Basics of Materials Science

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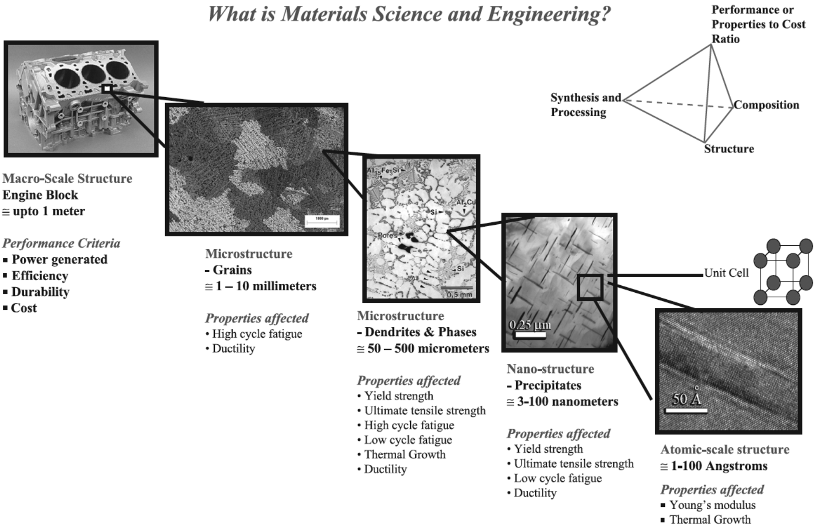
Outline

- Understanding scales
- Classification of materials
- Bonding in molecules and solids

MSE tetrahedron & scales: Mechanical properties

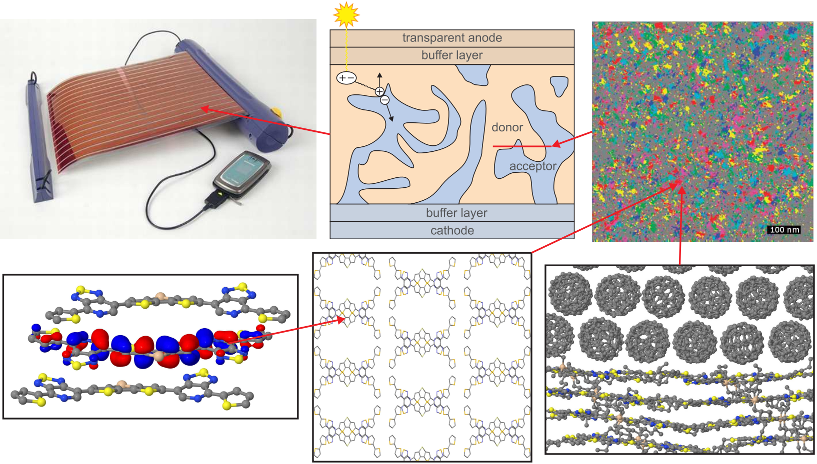


A real-world example of important microstructural features at different length-scales, resulting from the sophisticated synthesis and processing used, and the properties they influence. The atomic, nano, micro, and macro-scale structures of cast aluminum alloys (for engine blocks) in relation to the properties affected and performance are shown. The materials science and engineering (MSE) tetrahedron that represents this approach is shown in the upper right corner.

(Illustrations Courtesy of John Allison and William Donlon, Ford Motor Company)

MSE tetrahedron & scales: Electronic properties

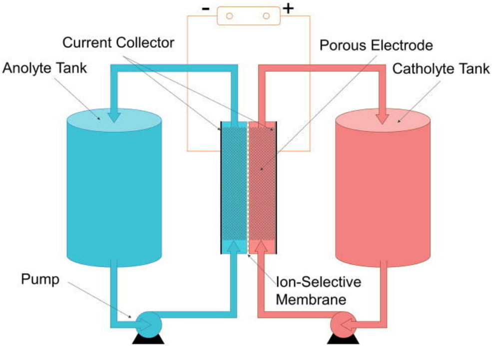
Focusing on structure-property relationships



Synthesis & Processing – **Structure** – **Properties** – Engineering & Technology

Understanding scales: example

Developing membrane for redox flow battery at CEST CREI

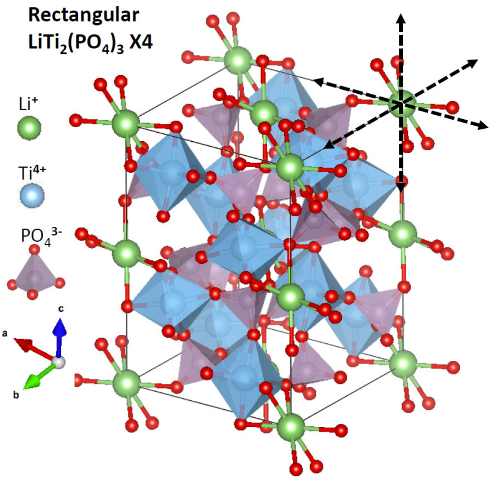


Key properties to optimize:

- High ionic conductivity and low electronic conductivity
- Selectivity
- Chemical and mechanical stability

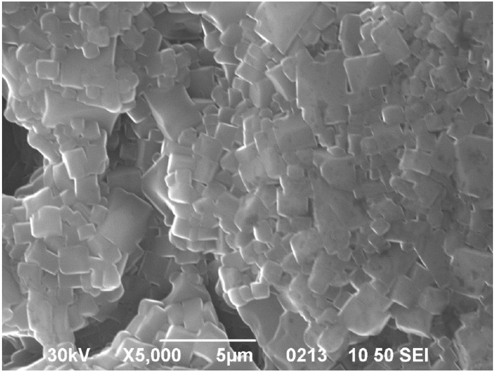
Atomistic scale: optimize chemical composition

$Li_{1+x}Al_xGe_yTi_{2-x-y}(PO_4)_3$



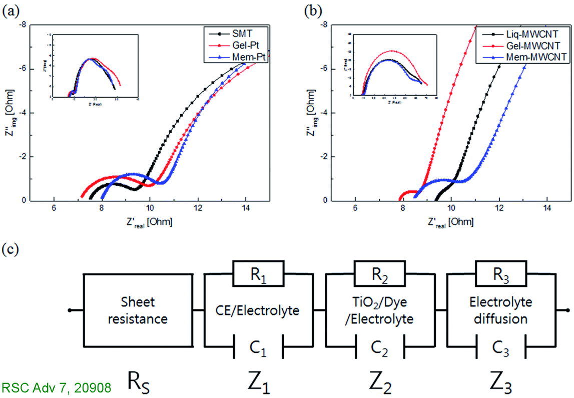
Single-material scale: optimize synthesis and morphology

(solid state synthesis, X-ray, TEM)



Device scale: test and optimize device architecture

(electrochemical impedance spectroscopy, aging tests, device modeling and engineering)



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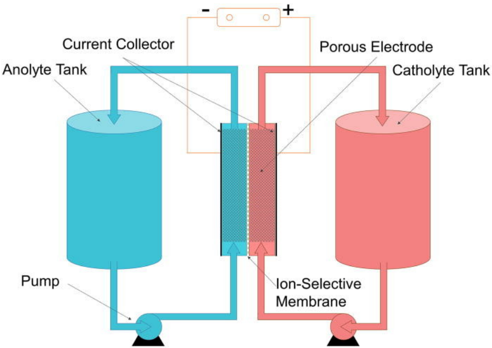
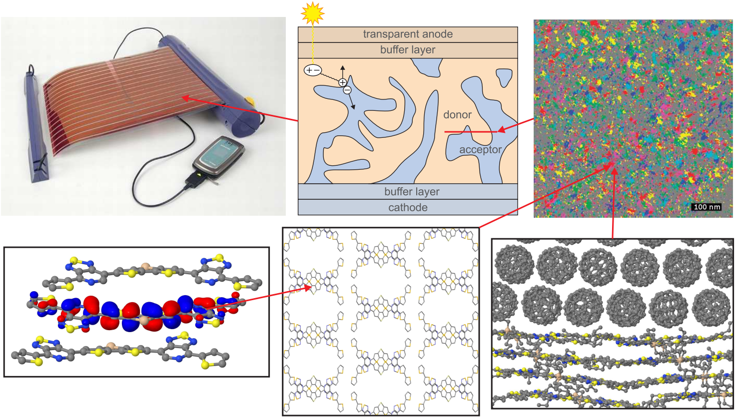
Real membrane in redox flow battery



- High ionic conductivity and low electronic conductivity
- Selectivity
- Chemical and mechanical stability

Now you can patent it, then consider other parts, upscale and commercialize

Understanding scales: Discussion



Let's try to address

1. Sunlight harvesting efficiency
2. Efficiency of charge separation
3. Degradation and aging

Classification of materials

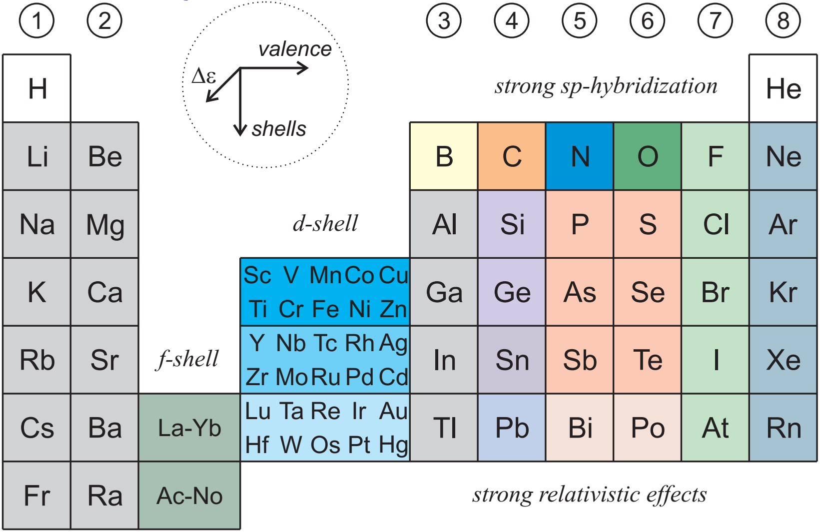
You want to create a device – how will you find suitable materials?

You are always searching in a specific class of materials.
Materials are classified at least by

- chemical composition
- structure (various scales)
- properties
- processing technology

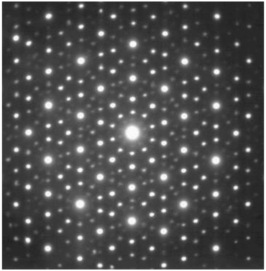
and also by availability, recyclability etc.

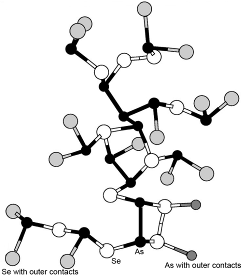
Classification by composition

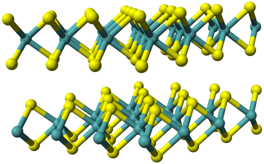


Organic, sp-metals – transition metals – actinides, oxides – nitrides – halides, light/heavy elements, electron-rich, average valence 4/5, abundant/rare/critical, radioactive, . . . ~~toxic/biocompatible~~

Classification by structure







- crystals, polycrystals, quasicrystals, liquid vs plastic crystals
- liquids, glasses, amorphous solids, (gases)
- surfaces and low-dimensional materials, polymers
- mixtures and nanostructured materials: solutions, blends, composites, interfaces, sandwich structures, adsorbates, thin films ...

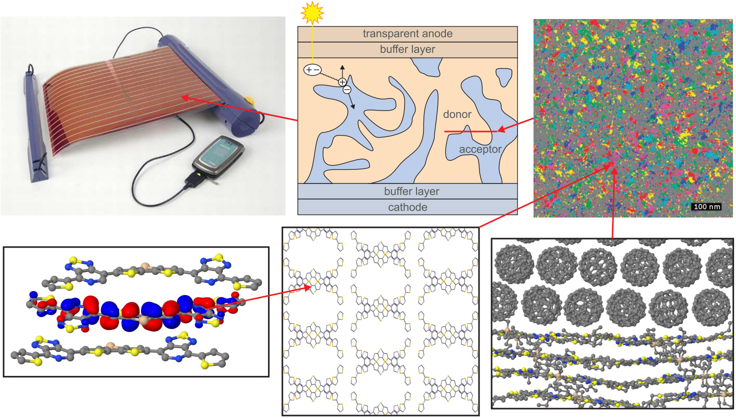
Classification by properties

- mechanical properties: metals, plastics, ceramics, composites, fibers, glasses
- electronic structure: metals, semimetals, semiconductors, insulators, superconductors, graphene, topological insulators
- electrical conductivity: metals, semiconductors, insulators, superconductors, solid ionic conductors, electrolytes
- electric properties: dielectrics, high-k dielectrics, piezoelectrics, pyroelectrics, ferroelectrics, capacitors
- optical properties: light absorbers, conducting transparent oxides, chiral crystals, nonlinear optical materials
- magnetic properties: ferromagnetics, magneto-optical materials
- nanoporous materials: zeolites, clathrates

Classification by processing technology

- metallurgy: metals and alloys
- 3D printing: plastics, metals, ceramics; rapid prototyping, additive manufacturing
- semiconductor fabrication plants (fab): "2D printing"; classical semiconductors
- solution processable: molecules, polymers, ionic solids; spin coating, inkjet printing; R2R processing, printed electronics
- chemical vapor deposition (CVD): highest quality solids
- graphene and 2D: special processing
- biosynthesis/biodegradation: biomolecules and biopolymers; low-cost, low-energy, environment-friendly

Classification of materials: Discussion



Let's try to find material for

1. Active layer: donor and acceptor
2. Buffer layers
3. Electrodes: top and bottom

Bonding in molecules and solids

Given a chemical composition:

- Predict structural preferences
- Estimate binding (cohesion) energy: $E(\mathrm{A}) + E(\mathrm{B}) - E(\mathrm{AB})$
- Speculate on functional properties

Sets of simple rules and concepts:

- Atomic radii (metallic, covalent, ionic, vdW)
- Close packing for isotropic interactions
- Valence shell electron pair repulsion (VSEPR) theory for molecules and covalent solids
- Huckel's rule for π-conjugated molecules
- Hume-Rothery rules for alloys
- ...

Accurate empirical potentials (force fields, EAM, EIM, COMB)

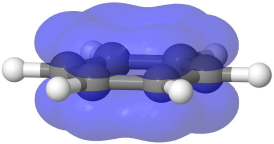
Bonding: Basic interactions – let's discuss

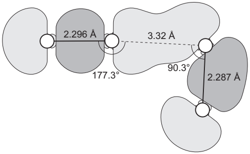
- covalent
- ionic
- metallic

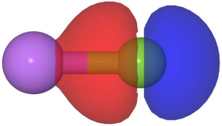
- steric
- donor-acceptor
- residual chemical

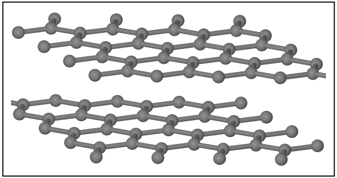
- hydrogen

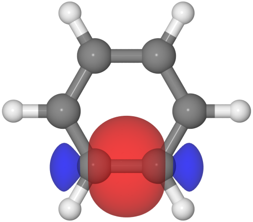
- electrostatic
- London dispersion
- medium mediated
- other physical

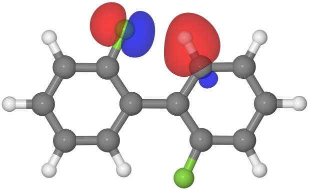












H_2O vs SO_2 vs CH_4

Summary and Resources

See summary here

- Wikipedia
- Crystal structures
- Crystallography Open Database
- References: structure, bonding
- Textbooks