Materials Science

Materials science combines the fields of chemistry, physics, engineering, biology, and computer science to create materials for a healthier and more sustainable future.

many people

The most useful thing ~~you've~~ never heard of.

Almost everything around you is made of different materials.

Materials scientists investigate how materials are made, figure out how they can be changed and improved, and engineer entirely new materials.

Materials Science

Understand/Manipulate:

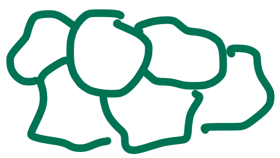
Structure
Properties
Processing
Performance
Characterization

Across length and time scales

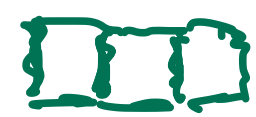
Materials Science: Structure

What do you think "Structure" refers to, and how to determine or describe it?

Ordered vs. disordered – repeating unit? Å (0.1 nm) time? → evolution?

Grains  10–100 μm

Temperature effects on structure – concrete, polymers, solid/liquid, phase transformations

Dislocations – line direction, Burgers vector / cell structures 

Crystal structure

Chemical structure, atomic bonding

Point defects

Cracks

Metamaterials (mm scale)

Composite structure

Protein structure

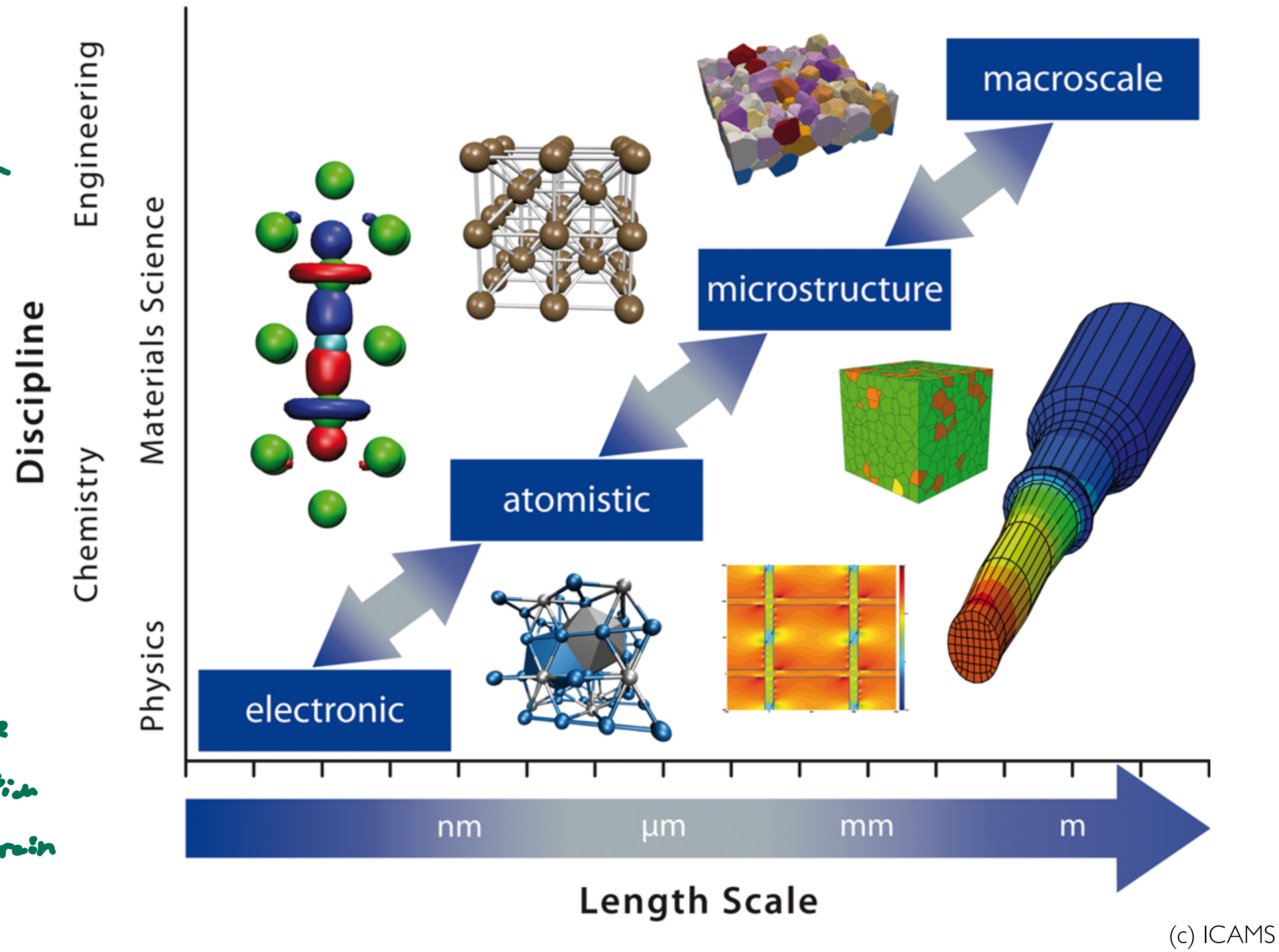
Precipitates – second phase

Materials Science: Structure

Describing microstructure:

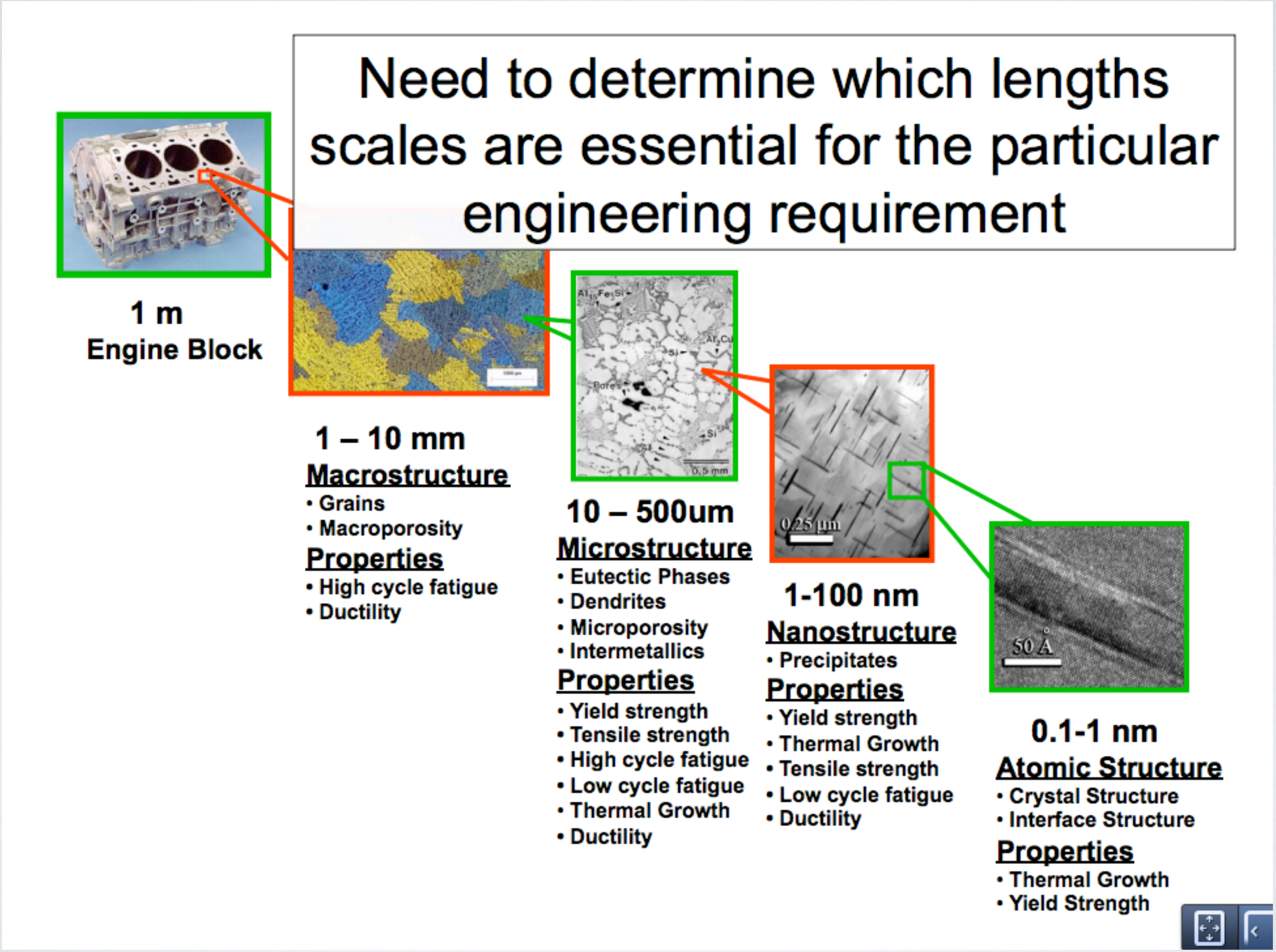
Grain structure
- size distribution
- texture (orientation distribution)
- grain boundary shape, type

Secondary phases / precipitates
- chemistry in each phase
- shape precipitates
- dendrite structure
- spatial distribution
- internal stress / strain
- volume fraction
- size distribution - orientation - spatial correlation - time evolution



- Materials Science is inherently "multi-scale" and "multi-physics"
- Different effects important on different length/time scales
- Impossible to tackle everything on atomistic level

Structure is multiscale



Materials Science: Structure

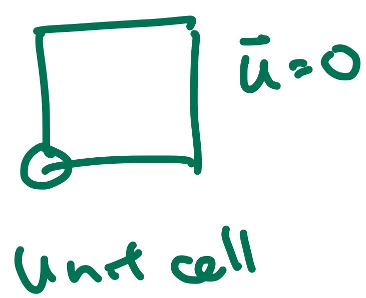
- Atomic Structure: If periodic, we use Bravais lattice+basis

14

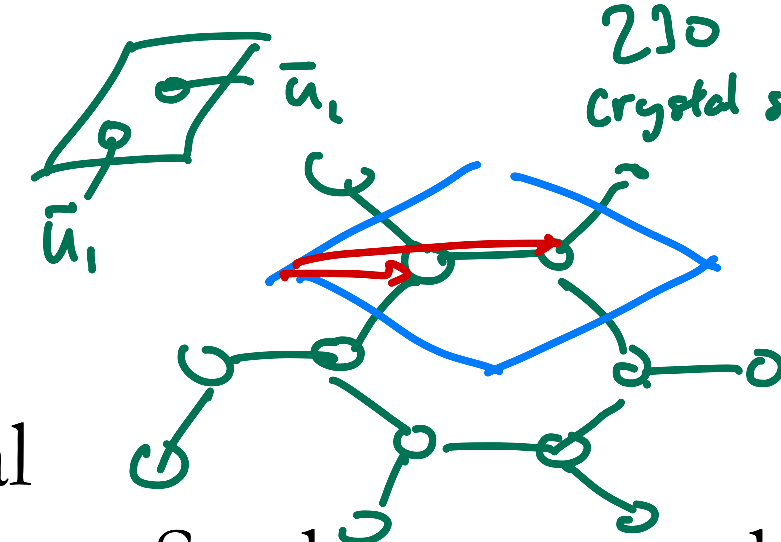
lattice – periodic, repeating unit in 2D or 3D

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 + \vec{u}_i$$

lattice vectors (under $n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$); basis (under $\vec{u}_i$)



230
crystal structures



- Many polymorphs even for one material
- Many systems are disordered/have defects. So they get much more complicated!
- True across many different length scales

Materials Science: Properties

Think of some examples for materials properties!

Toughness (energy absorbed before fracture)

Ductility (strain until failure)

Malleability

Melting point (temperature of solid-liquid phase transformation)

Fatigue limit (# of cyclic loads until failure)

Density (mass/volume)

Yield strength (onset of plastic deformation)

Electrical conductivity $\sigma \rightarrow$ current density = (conductivity) × field

Flourescence (response to EM radiation to re-emit photons)

Thermal conductivity (heat flux = σ × thermal gradient)

Glass transition temp

Magnetic temperature

Magnetization

Susceptibility

Emissivity

Permeability

Diffusivity

Heat capacity

Opacity

Taste

Elastic constants

Viscosity ($\dot{\gamma} = \frac{1}{\eta}\tau$)

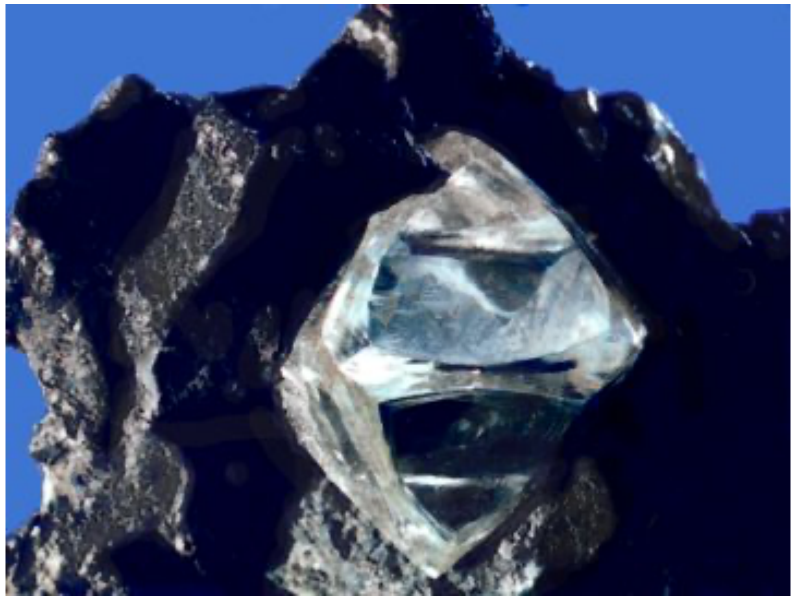
Band gap

Mobility

Materials Science: Properties

Material	electrical resistivity at 20°C (ohm-meter)
Aluminum	2.65×10^{-8}
Carbon (graphite, in plane)	5.0×10^{-6}
Germanium	4.6×10^{-1}
Silicon	2.3×10^{3}
Carbon(diamond)	10^{12}

temperature dependent



Materials Science: Characterization

Methods to provide information about properties and structure

What are characterization techniques?

Optical imaging
UV Spectroscopy
Tensile test
Hardness / Indentation
Scanning Electron Microscopy
Creep test
DMA (Dynamical Mech. Analysis)
Transmission electron microscopy
Scanning tunneling microscopy
Rheology (viscosity)

Atomic force microscopy

X-ray diffraction
X-ray tomography
Grazing incedent (sp?) X-ray spectroscopy
Infrared Thermography (emissivity)
Neutron diffraction
Raman spectroscopy
Conductivity measurement
Mercury intrusion (porosity)
Thermal gravimetric analysis
Differential scanning calorimetry
Density (Archemedes?)
Mass spectroscopy

DFT

Materials Science: Characterization

	Apply	Measure
Compressibility $\kappa = \left(\frac{\Delta V}{V}\right)\frac{1}{P}$	Pressure P	Volume change ΔV
Magnetic susceptibility	Magnetic field	Magnetization
Resistivity	Electric field	Current
Thermal conductivity	Temperature gradient	Heat flow

Materials Science: Characterization

	Probe	Scatters off
Neutron	Neutron	Nuclei, spins
X-Ray	Photons	Electrons
Electron	Electron	Charge density

Atomic force microscope
Scanning Tunneling Microscope

Materials Science: Characterization Data Problems?

What data(-related) problems is characterization facing?

Reproducibility — Do we have a "representative volume element" — does our data represent the material?

Measurement resolution — High dimensional data — how do we visualize? How do we communicate?

Noise — Software to process the data

Inapplicable methods — Storing & managing the data
- dealing with a large (>>TB) amount of data
- sharing?
- processing & moving the data

Formatting — representing the data & documentation

Software sharing & co-editing (version control)

Sharing — people not being willing: proprietary issues, paper still being written, being busy, data in bad format, competition, ...
- data transfer speeds

non-disclosure agreements

technology transfer

Metadata — how to collect it, how to format it

Standards?

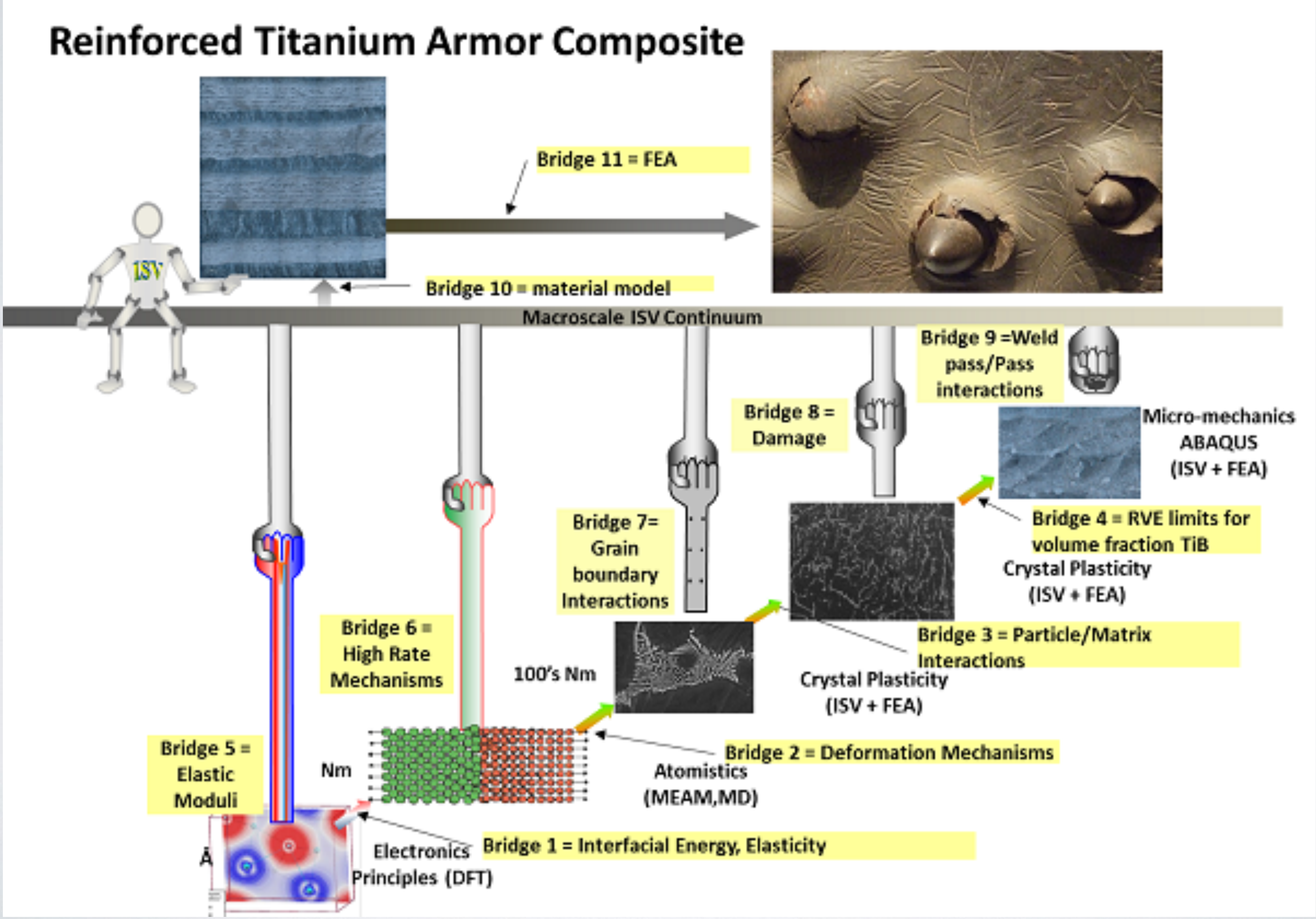
Materials Science: Data Problems?

- Collect enough data (with error bars) for:

Structure
Properties
Processing
Performance
Characterization

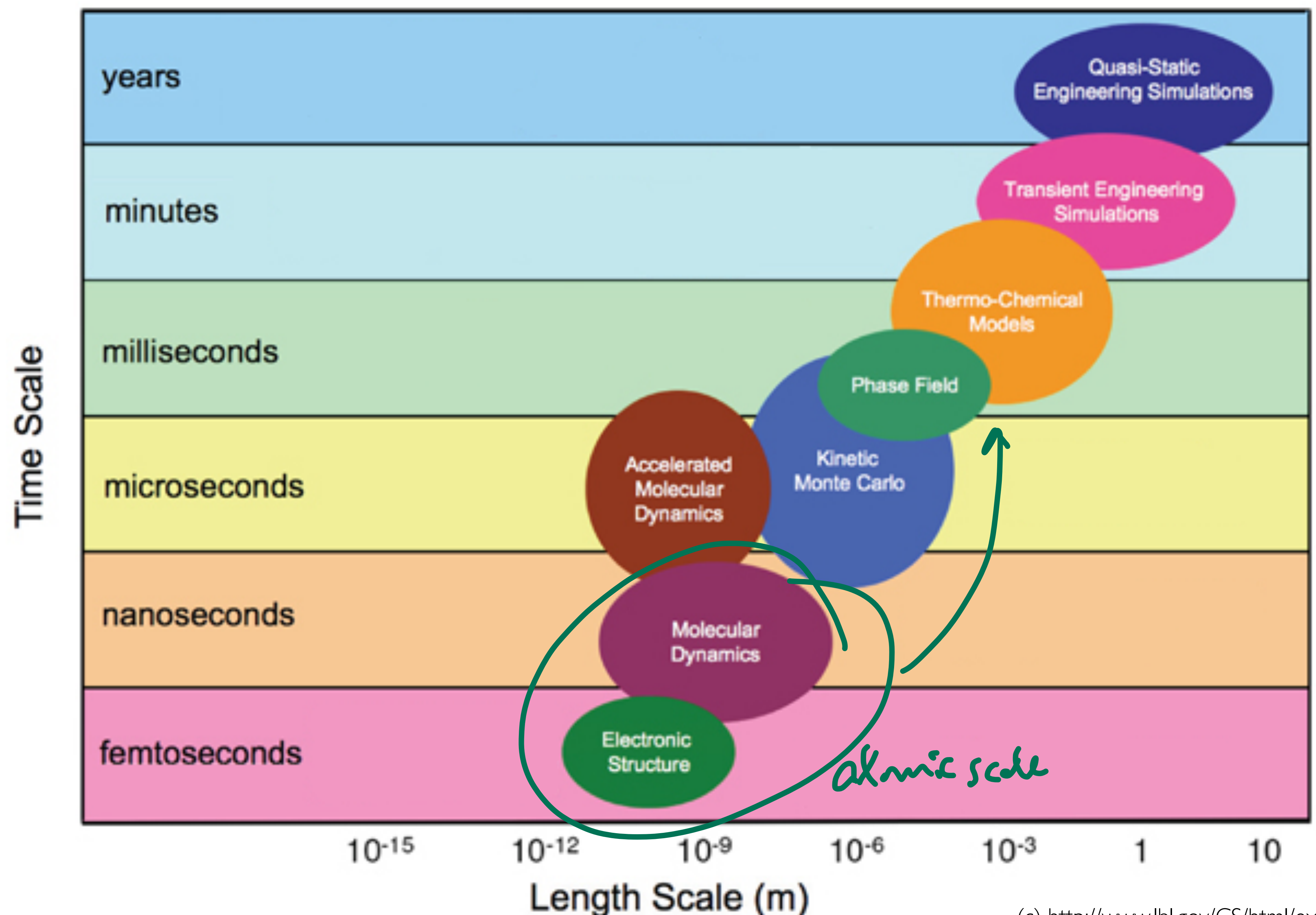
- Establish infrastructure to store all of this
- Establish ontologies that connect all of this
- Ultimately allow for predictions

And enabling ICME



https://icme.hpc.msstate.edu/mediawiki/index.php?title=File:Titanium_armor_length_scale_Bridging_plot.png&limit=20

Computational Methods: How?



(c) http://www.lbl.gov/CS/html/exascale4energy/nuclear.html

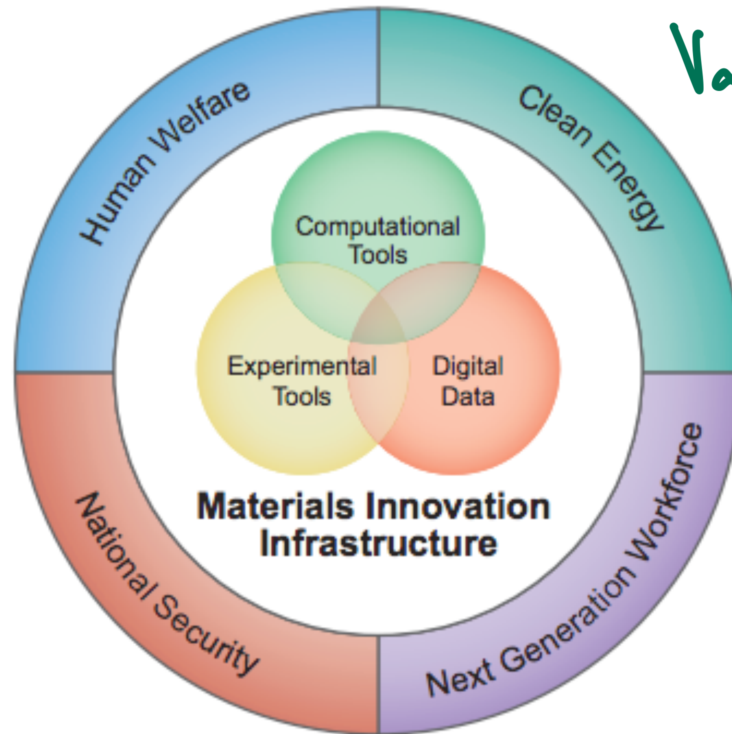
- Computational cost depends on level of accuracy
- Many different approaches/codes available (depends on goal)
- Interfacing different approaches can be difficult

Accelerating (Traditional) Materials Science

Verification: checking that a computation is solving a mathematical model accurately

bug checking

Convergence studies



(c) White House Materials Genome Initiative for Global Competitiveness (June, 2011)

Validation: does the mathematical model capture reality?

Comparison with experiments

define the domain of validation

- Experiment is/can be limited and/or expensive
- Simulations can complement the experiment
- Simulations are “easy” even for complex systems

- Validated computational models to perform:

prototyping	screening	materials selection
materials design	failure analysis	forensics
virtual analysis	optimization	reliability testing

Materials Science: Data Problems?

- Collect enough data (with error bars) for:

Structure
Properties
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Performance
Characterization

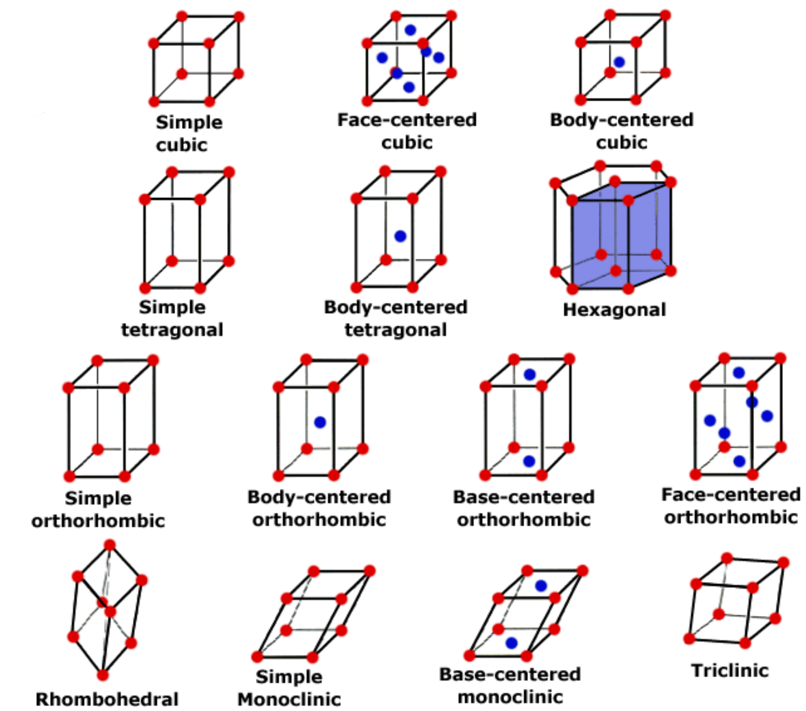
- Establish infrastructure to store all of this

- Establish ontologies that connect all of this

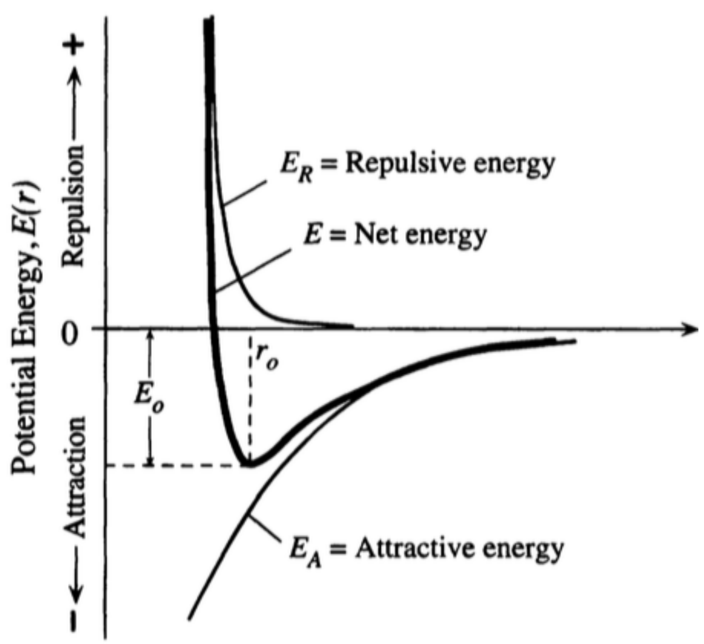
- Ultimately allow for predictions

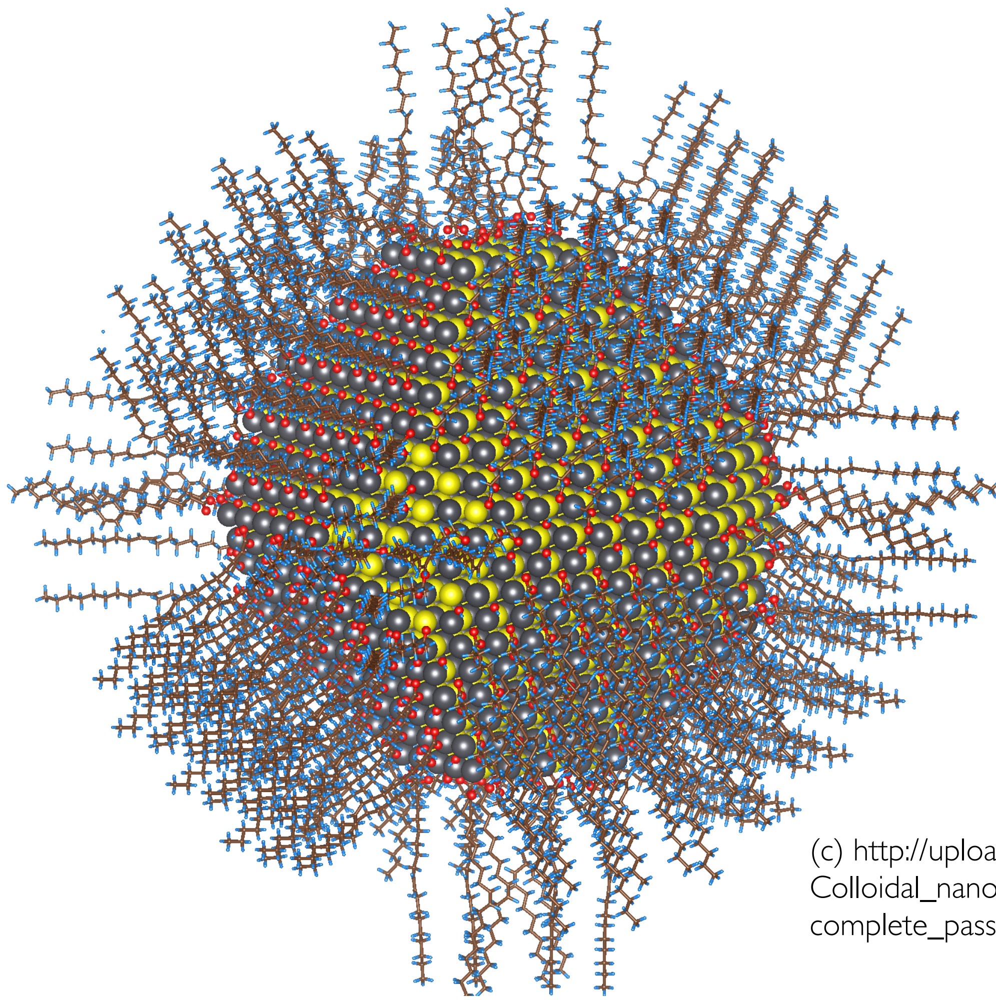
Computational Methods: Structural Properties

- Examples for Structural Properties:
  - Bonding/Crystal Structure
  - Surfaces
  - Interfaces
  - Passivation



(c) http://www.seas.upenn.edu/~chem101/sschem/bravais.gif





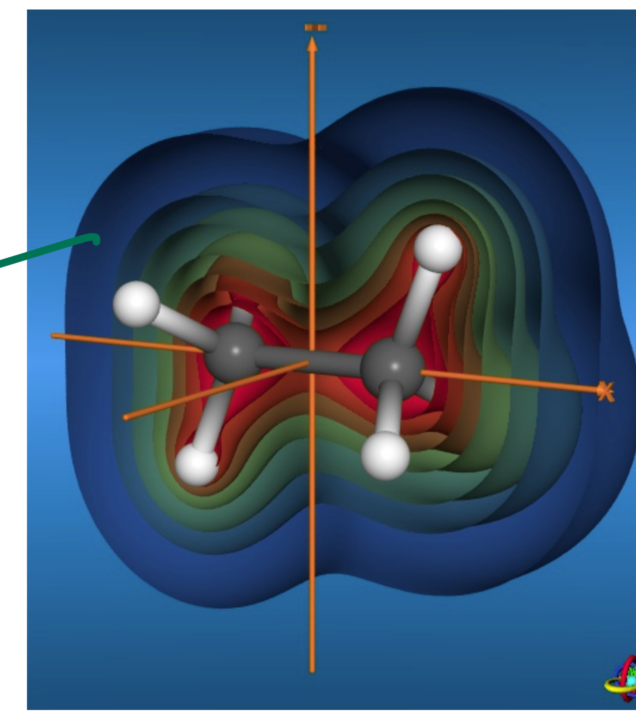
(c) http://upload.wikimedia.org/wikipedia/commons/7/75/Colloidal_nanoparticle_of_lead_sulfide_(selenide)_with_complete_passivation.png

Computational Methods: Structural Properties

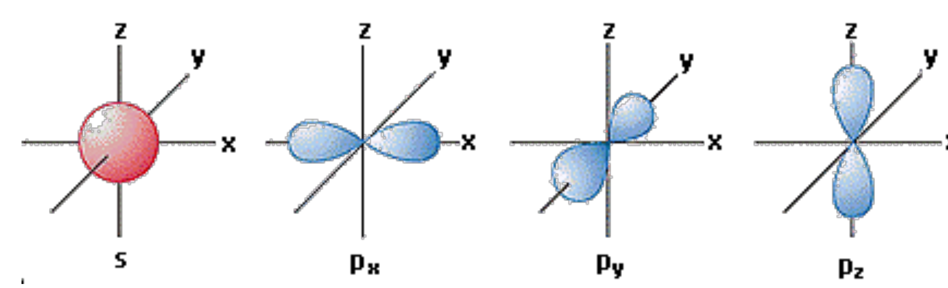
- Central Question: What is the arrangement of atoms that has the lowest total energy? → T ≈ 0K, otherwise requires free energy (U−TS)
- This is a quantum-mechanical problem, because electrons (and sometimes atoms) are quantum mechanical objects
- Electron described by wave function $\psi(\mathbf{r})$
- Probability of finding electron at position $\mathbf{r}$ in space:

$|\psi(r)|^2$

electron density contours



(c) http://csi.chemie.tu-darmstadt.de/ak/immel/tutorials/orbitals/molecular.html

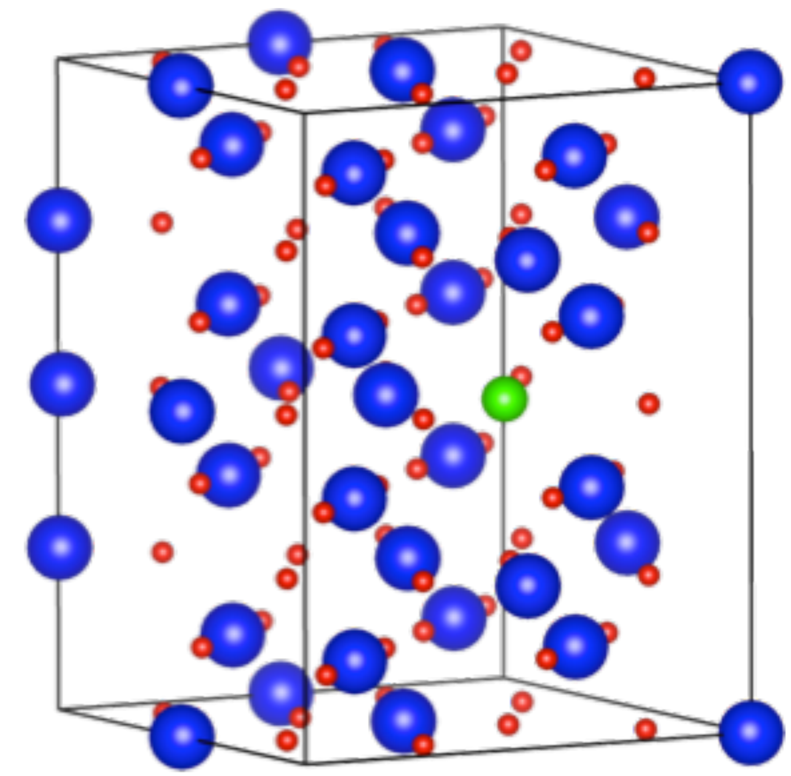


(c) https://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Images/hybrid1.gif

Computational Methods: Structural Properties

- Central Question: What is the arrangement of atoms that has the lowest total energy?

- What is the Hamiltonian?
  - kinetic energy $\left(\frac{1}{2}mv^2\right)$
  - Coulomb interaction $\frac{q_1 q_2}{r}$ $\quad r_{ij} := |\vec{r}_i - \vec{r}_j|$



$\hbar = e = m_e = c = 1$

$$H = -\sum_{i=1}^{N_e} \frac{1}{2}\nabla_i^2 + \sum_{i<j} \frac{1}{r_{ij}} - \sum_{i=1}^{N_e}\sum_{I=1}^{N_I} \frac{Z_I}{r_{iI}} - \sum_{I=1}^{N_e} \frac{m_e}{2M_I}\nabla_I^2 + \sum_{I<J} \frac{Z_I Z_J}{r_{IJ}} + (\text{external fields})$$

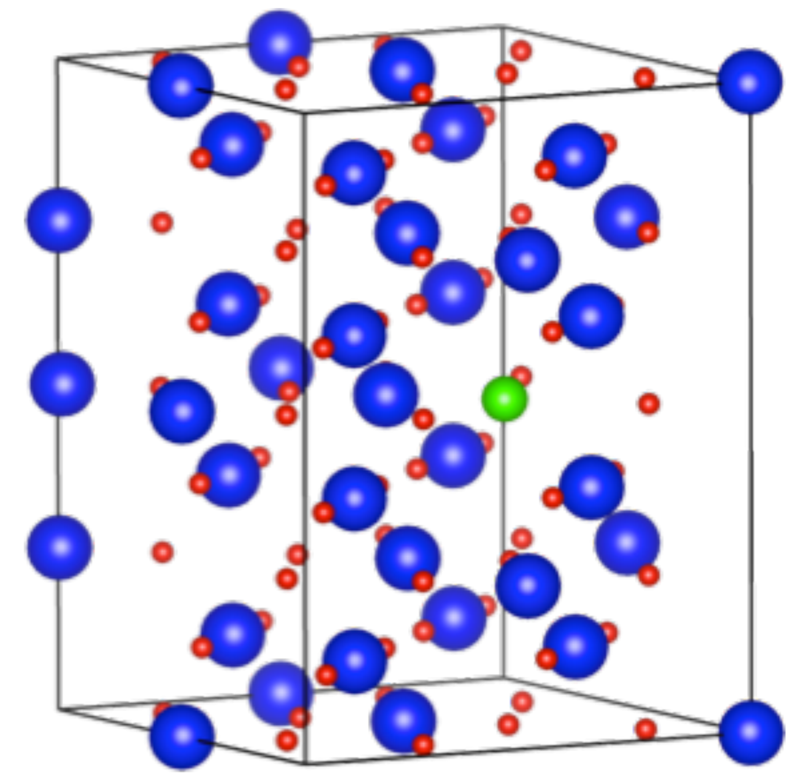
electron KE+interaction | electron+ion | ion KE + interaction | couples to individual particles

ion → nucleus + core e^-

Computational Methods: Structural Properties

- Central Question: What is the arrangement of atoms that has the lowest total energy?
- Very Common:
  1. Fix ions in some configuration **R**

     - classical, T=0K → no ion KE

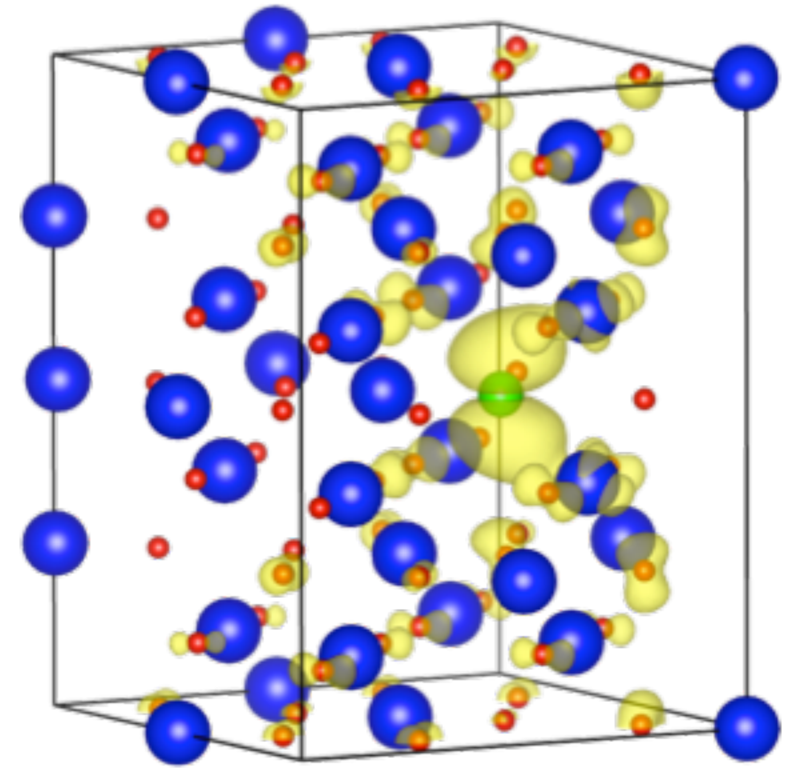


$$H = -\sum_{i=1}^{N_e} \frac{1}{2}\nabla_i^2 + \sum_{i<j} \frac{1}{r_{ij}} - \sum_{i=1}^{N_e} \sum_{I=1}^{N_I} \frac{Z_I}{r_{iI}}$$

electron KE+interaction electron+ion

Computational Methods: Structural Properties

- Central Question: What is the arrangement of atoms that has the lowest total energy?
- Very Common:
  1. Fix ions in some configuration **R**
  2. Solve electronic problem to get total energy and forces on atoms



Born-Oppenheimer approximation

$\hat{H}^{el}(\vec{R}_I)\psi(\vec{r}) = E(\vec{R})\psi(\vec{r})$

ion coord. electron coord.

$E_{TOTAL} = (\text{ion-ion}) + E(\vec{R})$

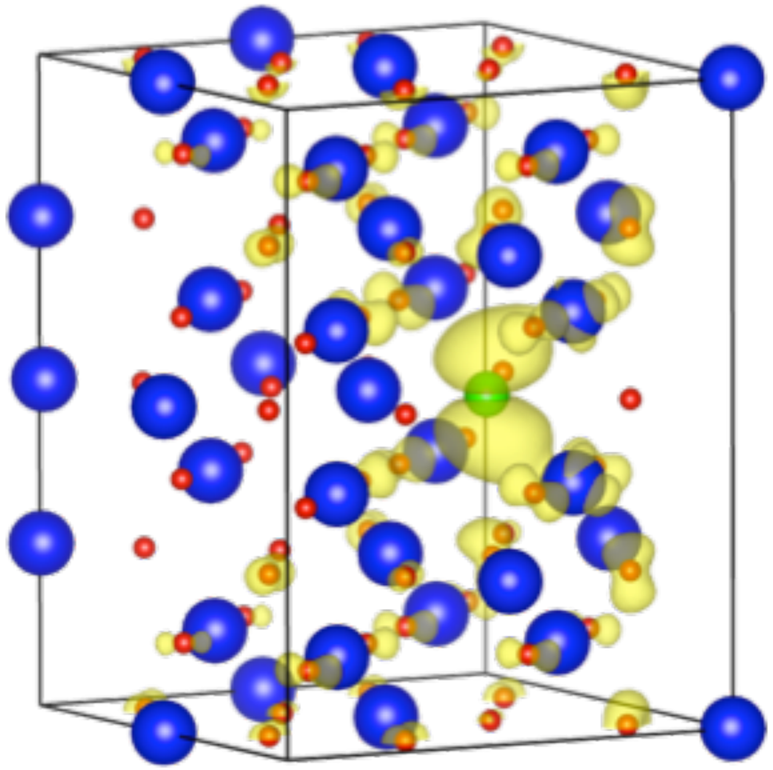
$\vec{F}(\vec{R}) = -\nabla_{\vec{R}} E_{TOTAL}$

$$H = -\sum_{i=1}^{N_e} \frac{1}{2}\nabla_i^2 + \sum_{i<j} \frac{1}{r_{ij}} - \sum_{i=1}^{N_e}\sum_{I=1}^{N_I} \frac{Z_I}{r_{iI}}$$

electron KE+interaction electron+ion

Computational Methods: Structural Properties

- Central Question: What is the arrangement of atoms that has the lowest total energy?

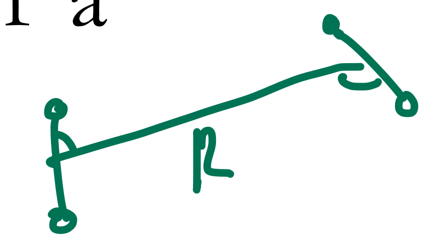


- Very Common:
  1. Fix ions in some configuration **R**
  2. Solve electronic problem to get total energy and forces on atoms
  3. Move atoms to **R'**, find configuration with smallest total energy

- Energy model $E(\mathbf{R})$
  - This would be the Schrödinger Equation:

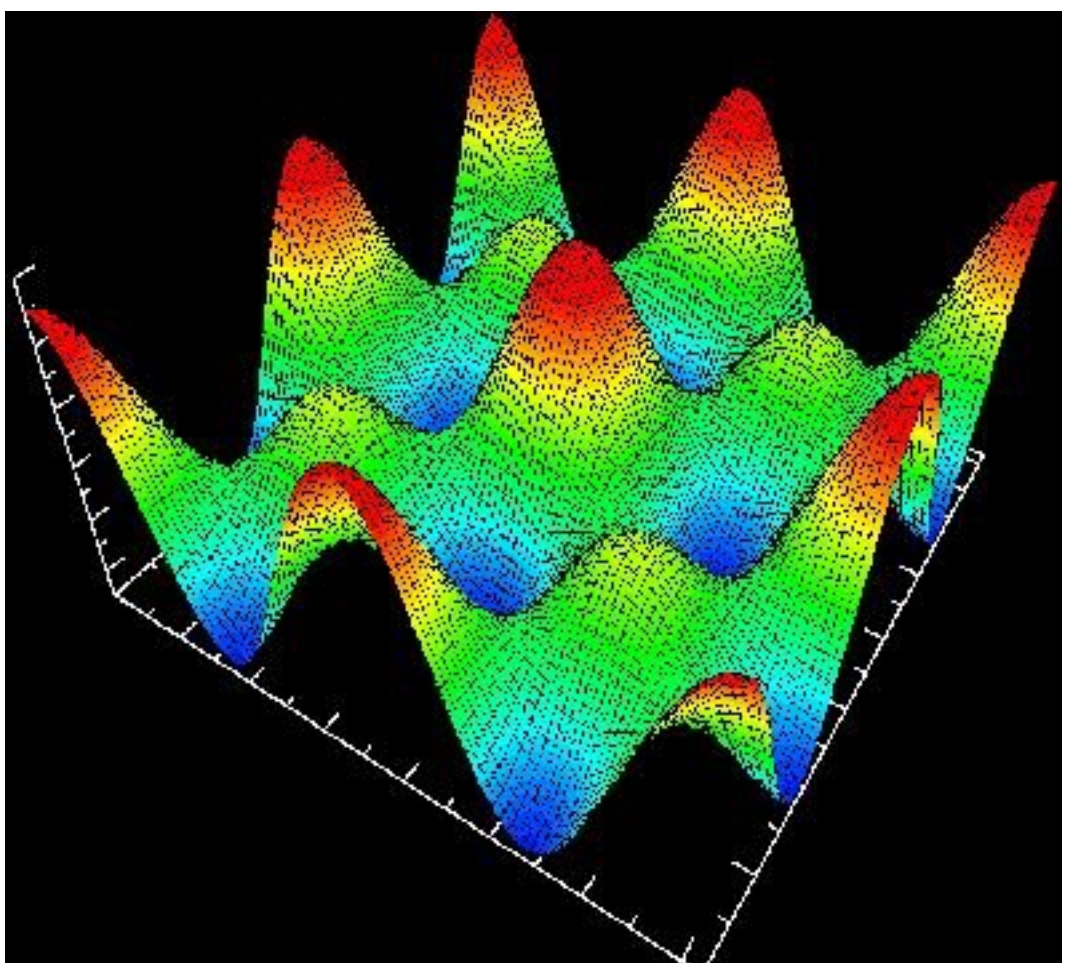
Bonding in Solids: Quantum Mechanics

- reality is complicated for solids, but the concept of a "potential energy surface" holds;



$$\hat{H}(\mathbf{R}, \mathbf{r})\psi(\mathbf{R}, \mathbf{r}) = E(\mathbf{R})\psi(\mathbf{R}, \mathbf{r})$$

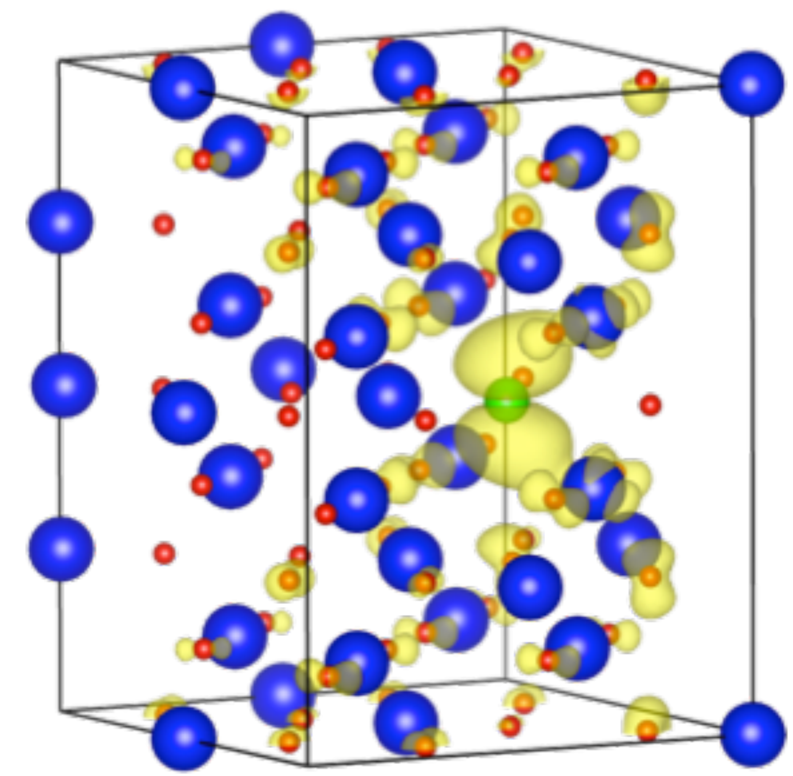
- example below shows the potential energy surface of H_2-H_2 molecule: $E(\mathbf{R})$



- 4 variables: one distance (between center of mass of two molecules) and three angles
- this is a 4D energy surface
- for plot: distance and one of the angles is fixed (not shown)
- pronounced directional dependence visible

Computational Methods: Structural Properties

- Central Question: What is the arrangement of atoms that has the lowest total energy?

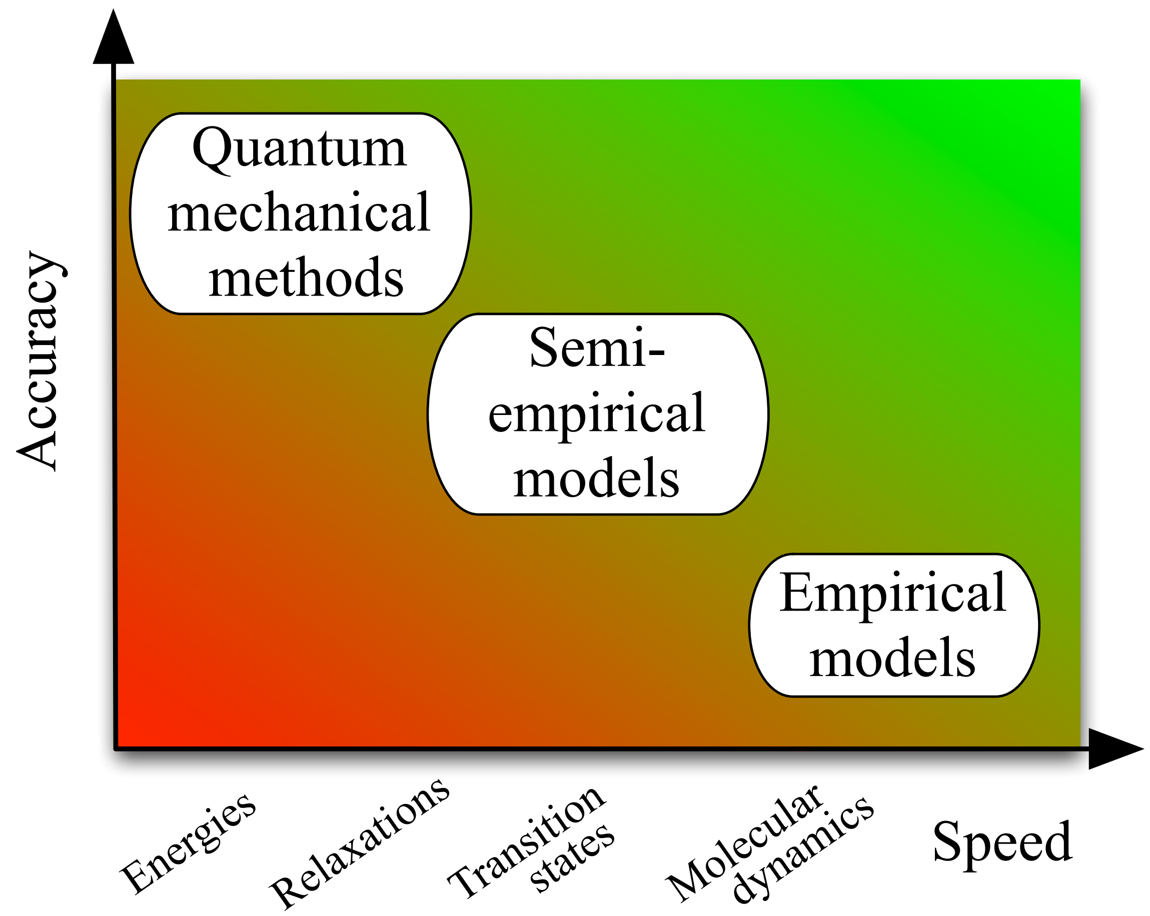


- Very Common:
  1. Fix ions in some configuration **R**
  2. Solve electronic problem to get total energy and forces on atoms
  3. Move atoms to **R'**, find configuration with smallest total energy

- Energy model $E(\mathbf{R})$
  - This would be the Schrödinger Equation
  - However: Cost of exact solution grows exponentially with number of electrons
  - Impossible for realistic systems

Computational Methods: Structural Properties

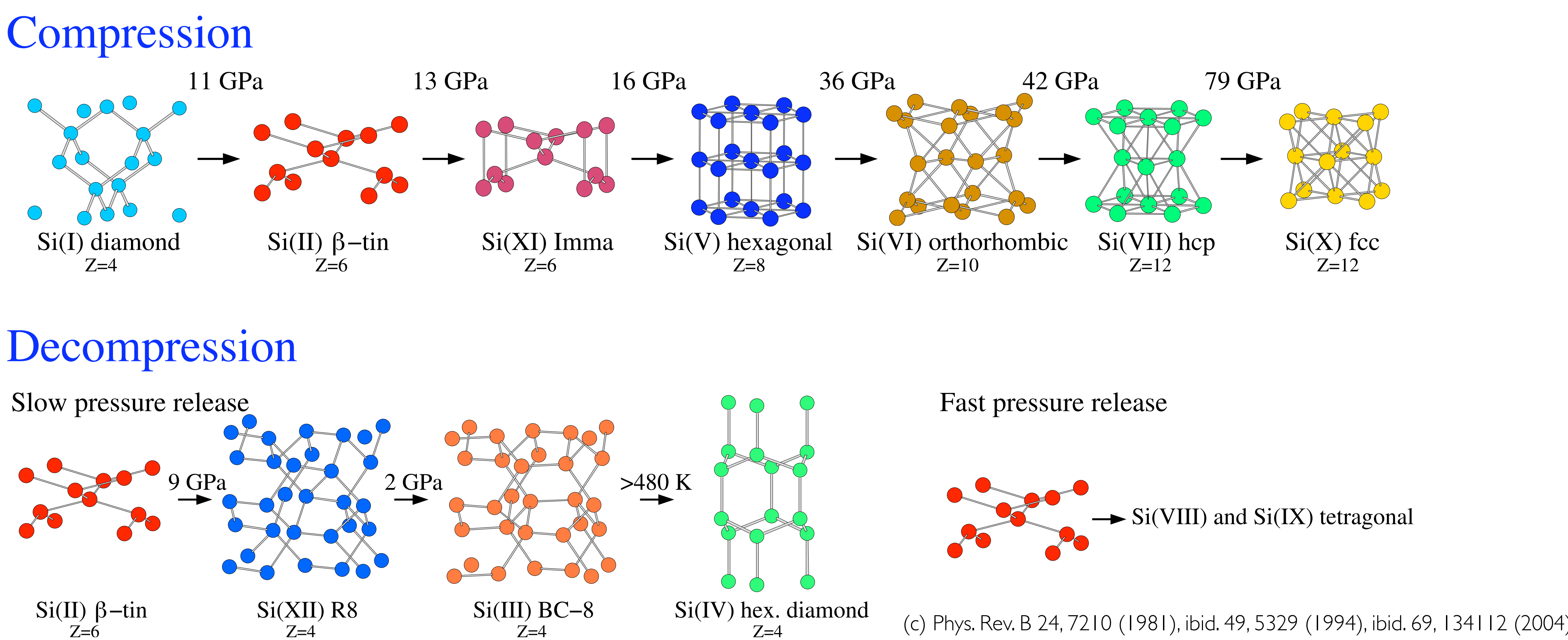
- Central Question: What is the arrangement of atoms that has the lowest total energy?
- Various Approximations possible:



- One (Approximate) Quantum Mechanical Method: Density Functional Theory

Computational Methods: Structural Properties

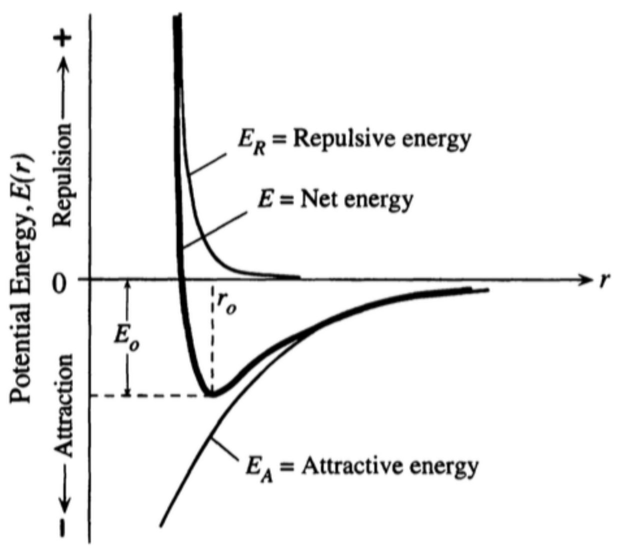
- Central Question: What is the arrangement of atoms that has the lowest total energy?
- Example: DFT correctly predicts different crystal phases of Si

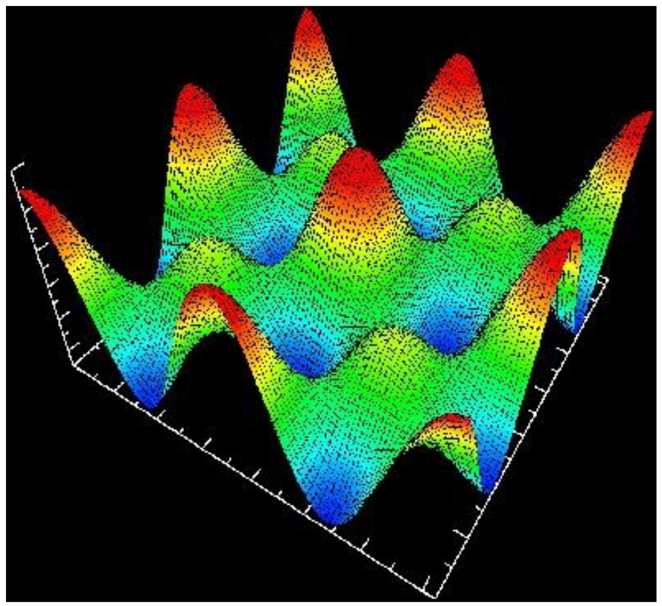


- Lattice parameters typically within 1% of experiment
- Depends on approximation for exchange-correlation functional

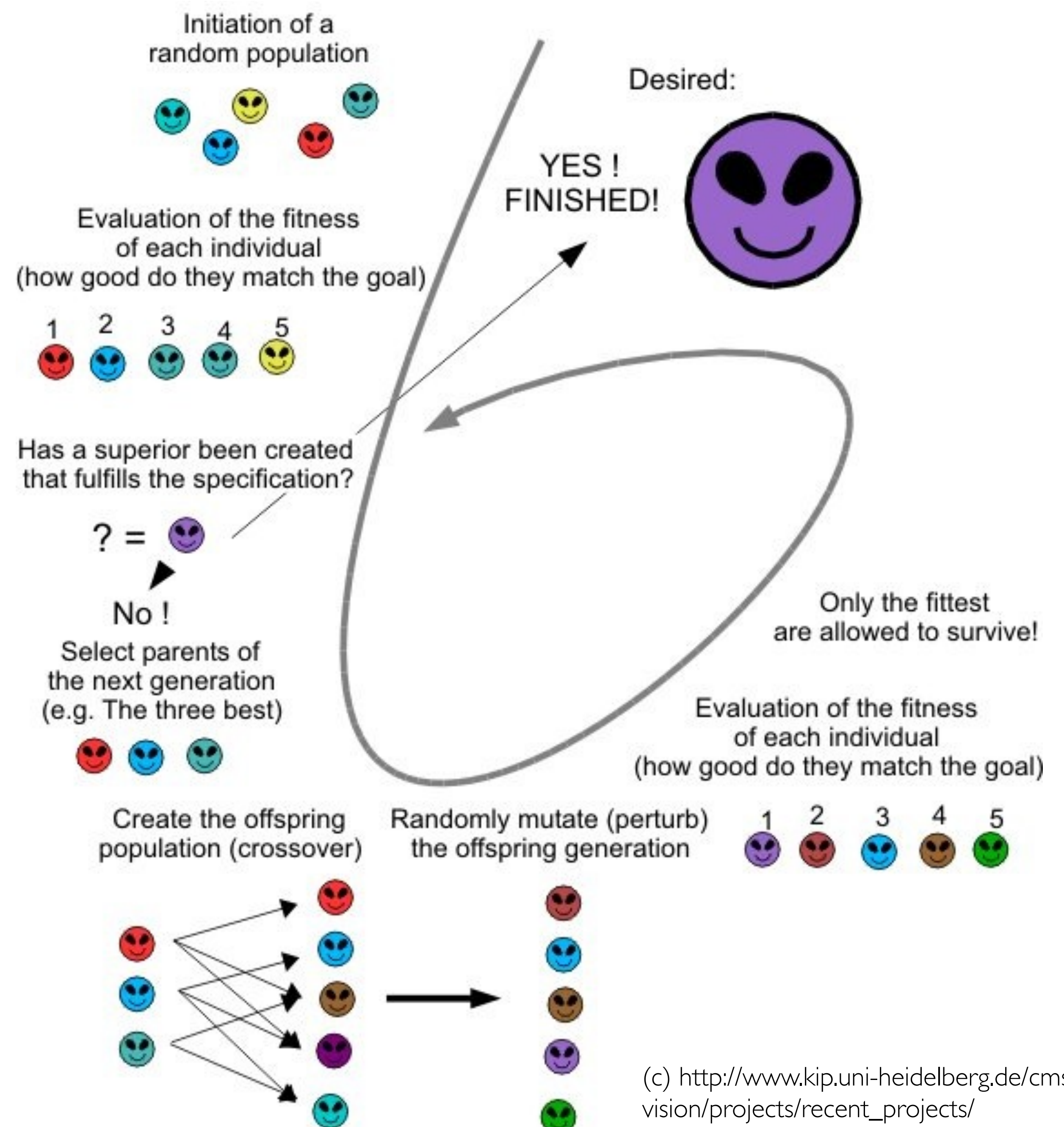
Computational Methods: Structural Properties

- Central Question: What is the arrangement of atoms that has the lowest total energy?
- Even if we know how to compute $E(\mathbf{R})$, we don't know how to answer this question yet!





(c) http://puccini.che.pitt.edu/frameset3b.html

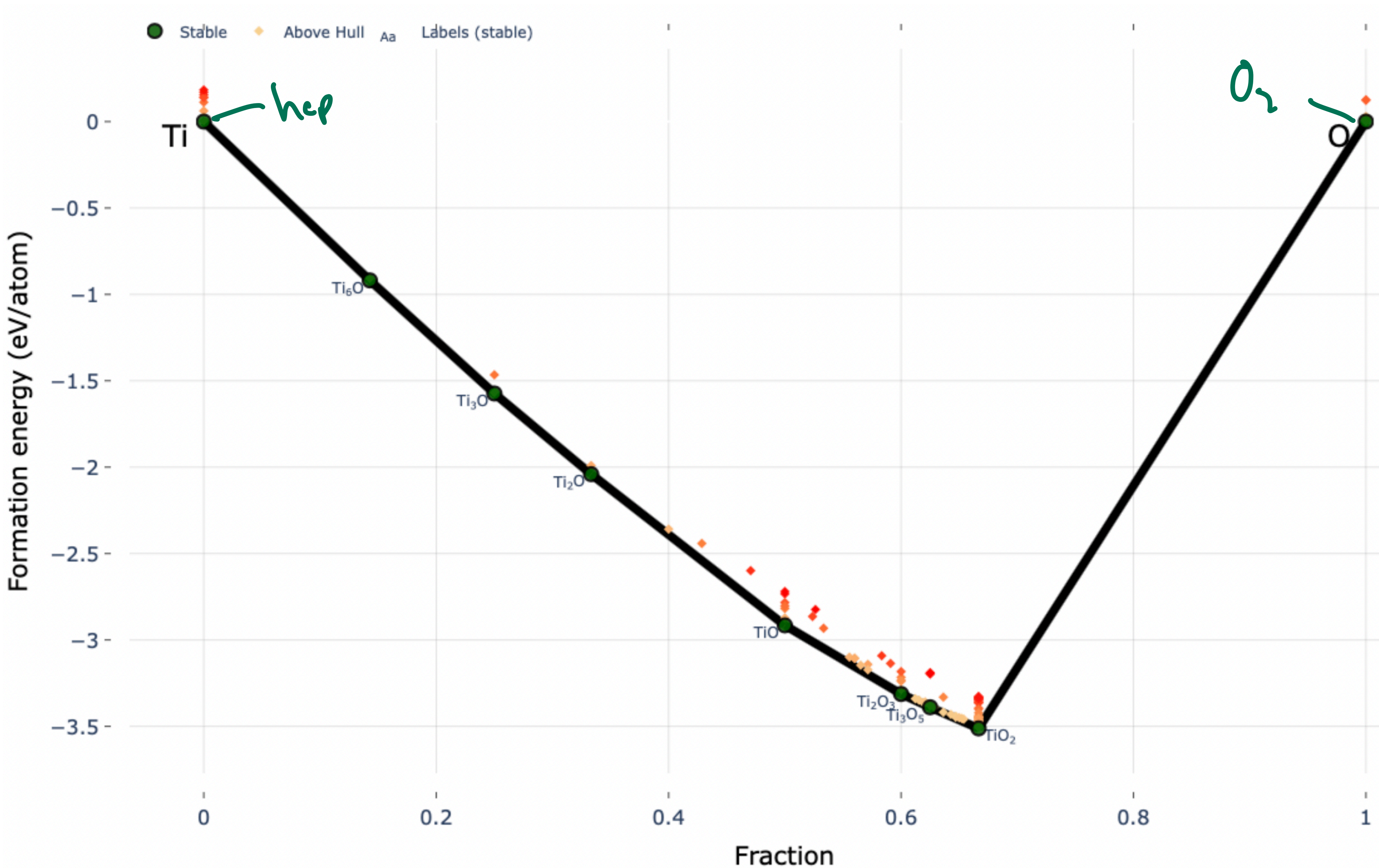


(c) http://www.kip.uni-heidelberg.de/cms/vision/projects/recent_projects/evolvable_hardware/evolutionary_algorithms/

- Many local minima!
- One possible technique: Evolutionary Algorithms/ Genetic Algorithms
- Applet

Computational Methods: Structural Properties

- Nowadays, (some of) this data is available in databases:



Computational Methods: Structural Properties

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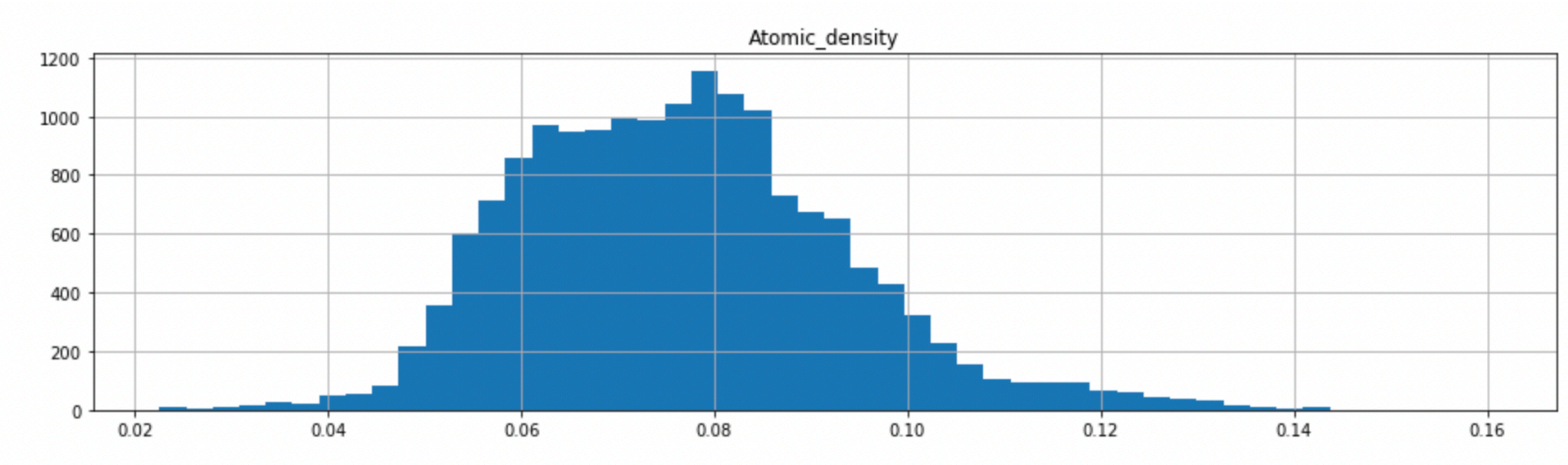
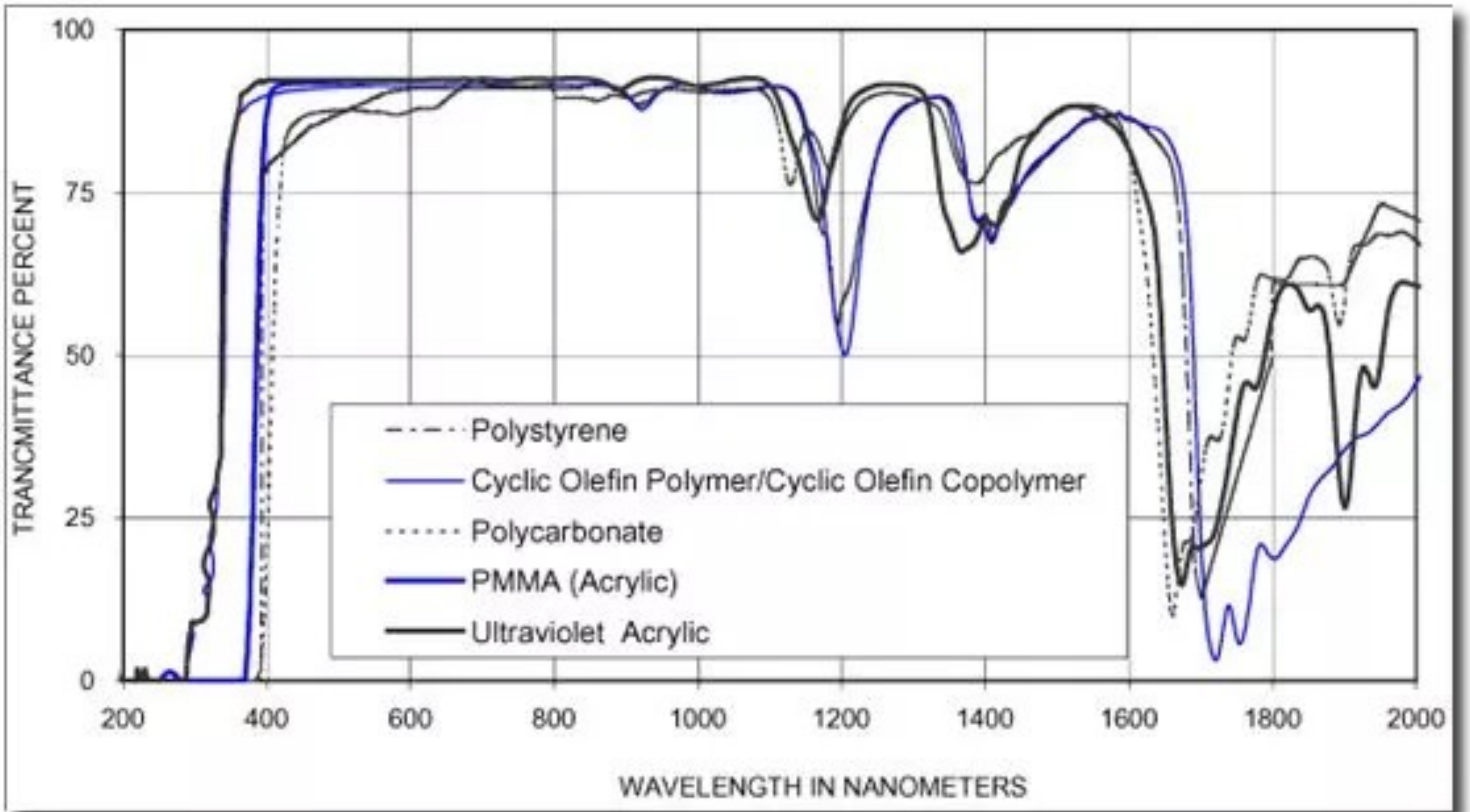


Materials Data: FAIR

- https://www.go-fair.org/fair-principles/

Materials Data: Schemas



- What information would have to be in the database?

Materials Data: Schemas

- https://nomad-lab.eu/prod/rae/docs/metainfo.html#starting-example
- https://doi.org/10.1557/mrs.2016.166