Materials for Energy

How pressing needs for innovative technologies demand new ways of creating materials and putting them together

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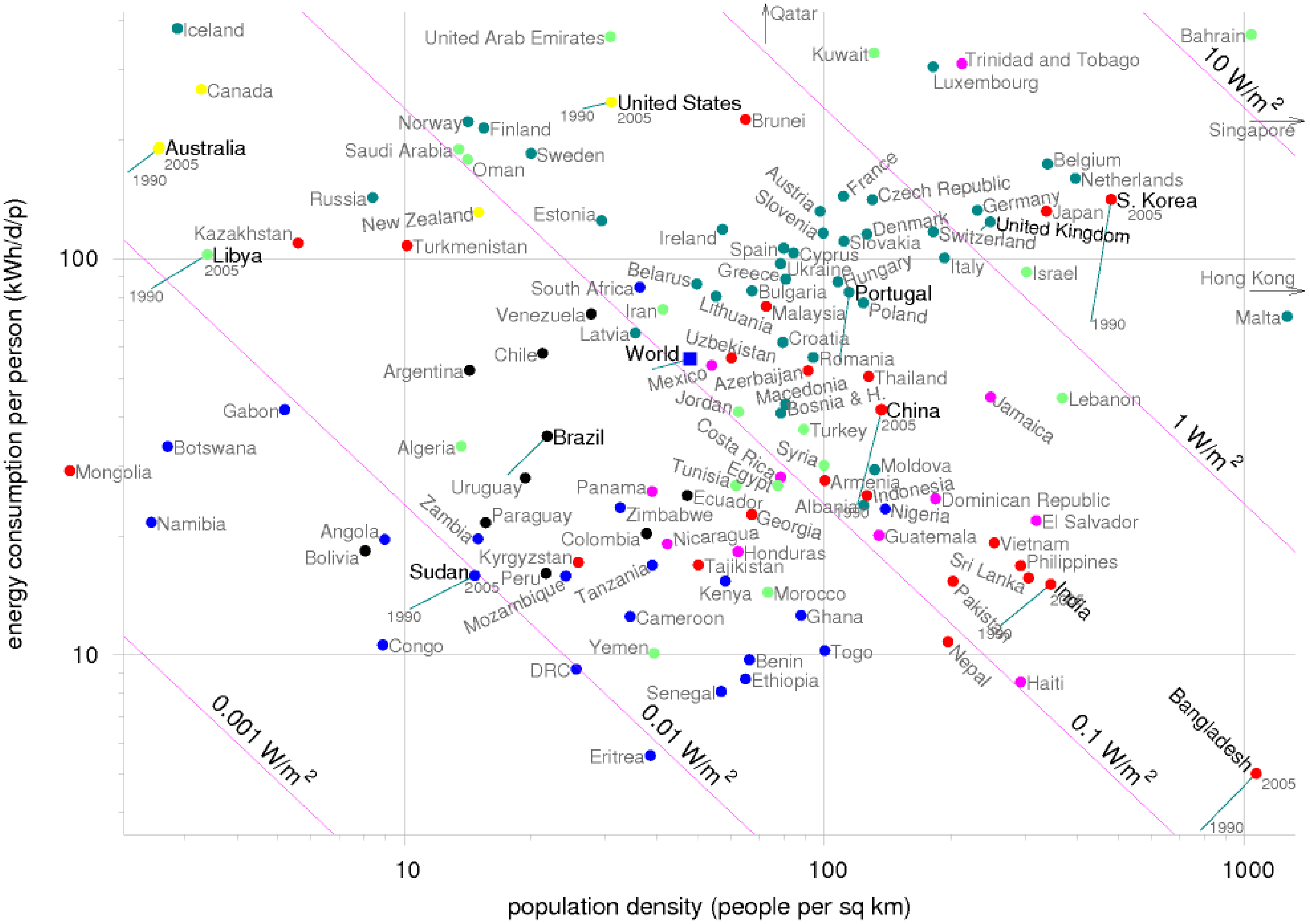
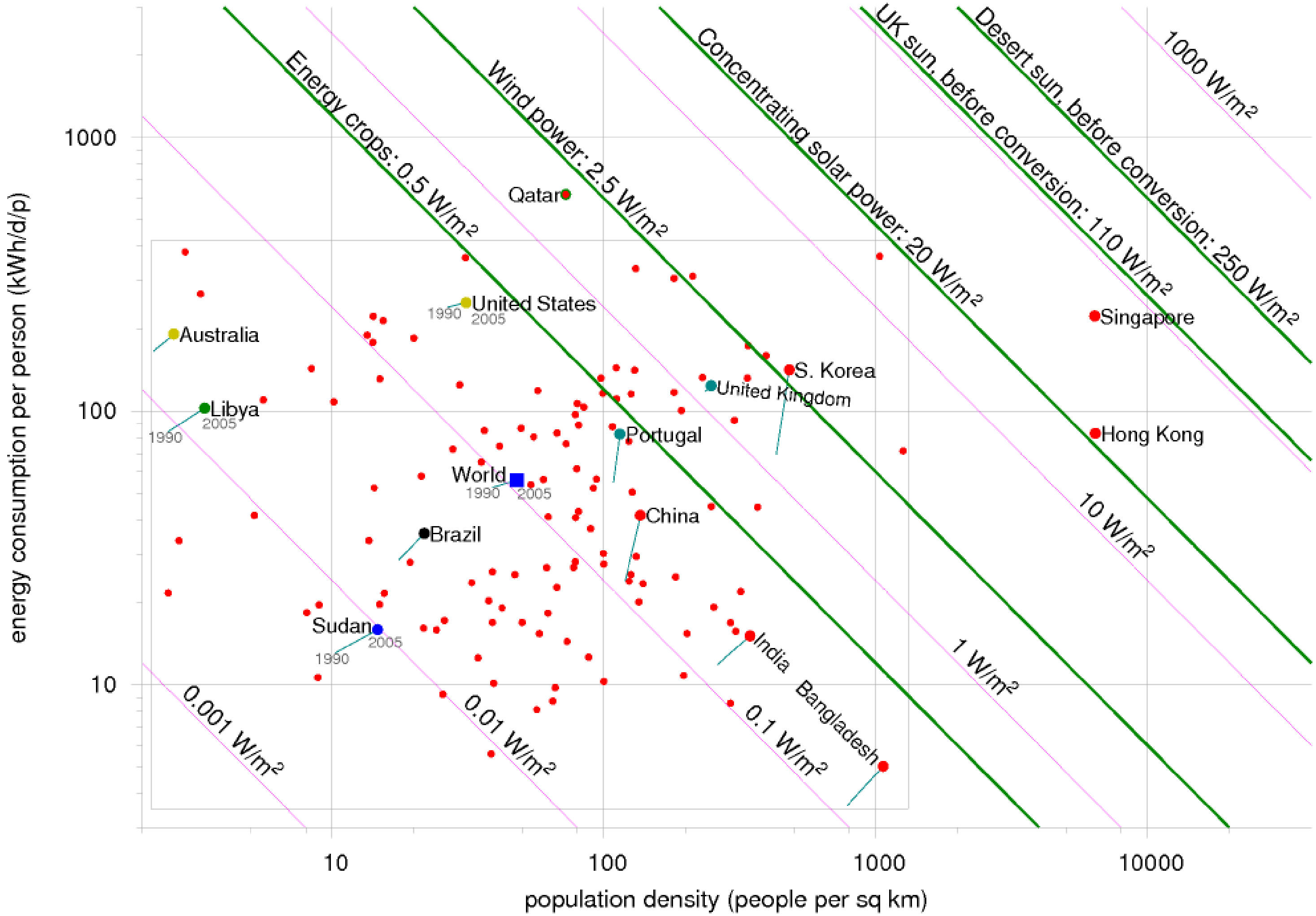
Secretary of Energy Advisory Board 17 April 2012

The scale of the challenge: Energy usage per m^2



Courtesy D J Mackay, UK DECC

Renewable deployments are country-sized



Courtesy D J Mackay, UK DECC

Challenges of Geography, Efficiency, and Cost

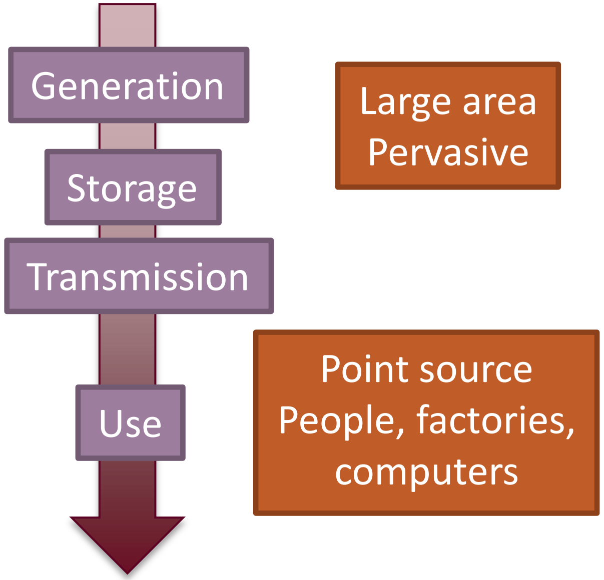
	Power density Watt/m^2
Full insolation Arizona desert	300
Concentrated solar power (desert)	15-20
Solar photovoltaic	5-20
Biomass	1-2
Tidal pools/tidal stream	3-8
Wind	2-8
Rainwater (highland)	0.3
US energy consumption (all sources)	0.3

In the US: Solar + wind + storage + grid infrastructure= sustainable economy

In the Global South: Solar + storage+ refrigeration+ lighting = education and healthcare

Transformative materials technologies for the electrified economy

- Solar PV for electricity generation (or solar to fuel)
- Ultracapacitors/batteries for electrical storage
- Superconductors for electrical transmission/motors
- Thermoelectrics for refrigeration/scavenging
- Light emitting diodes for electrical lighting
- Membranes for water purification/desalination


Generation
Storage
Transmission
Use

Large area
Pervasive

Point source
People, factories, computers

Point use is easier: smaller scale for fabrication, straightforward path to introduction
Large scale disruptive technologies are very hard

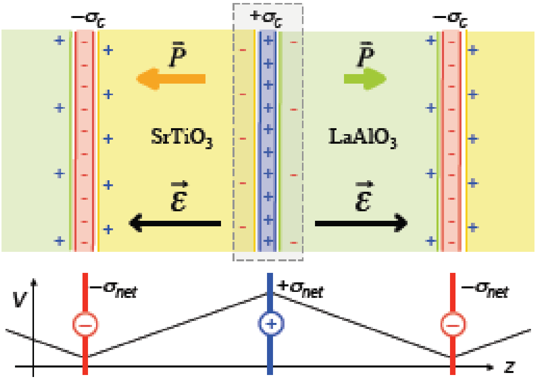
Aside from the grid, we have no examples of implementing wide scale “by the ton” electrical materials technology

Creating transformational technologies: nanoscience by the ton

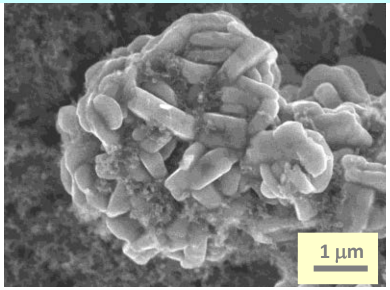
Four magic technologies: storage, photovoltaics, refrigeration and lighting depend on the science of *interfaces.*

- At least two orders of magnitude below optimal performance and too costly
- Devices are unnecessarily complicated, operation is poorly understood, and manufacturing difficult to control
- Major discoveries of new materials classes are rare and random
- There is no predictable path forward

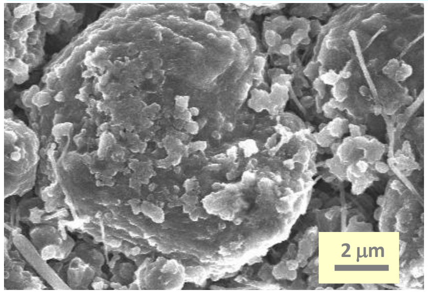
Model “solar battery” with storage density of order gasoline ?



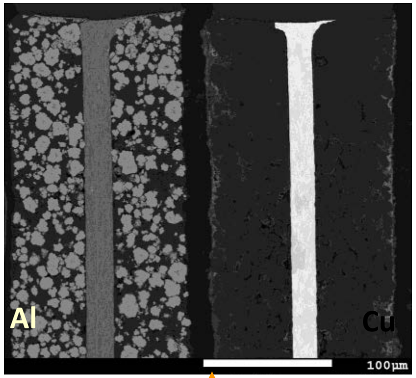
The cathode contains an oxide, carbon additives and PVdF binder



The anode contains graphite, carbon additives and PVdF binder



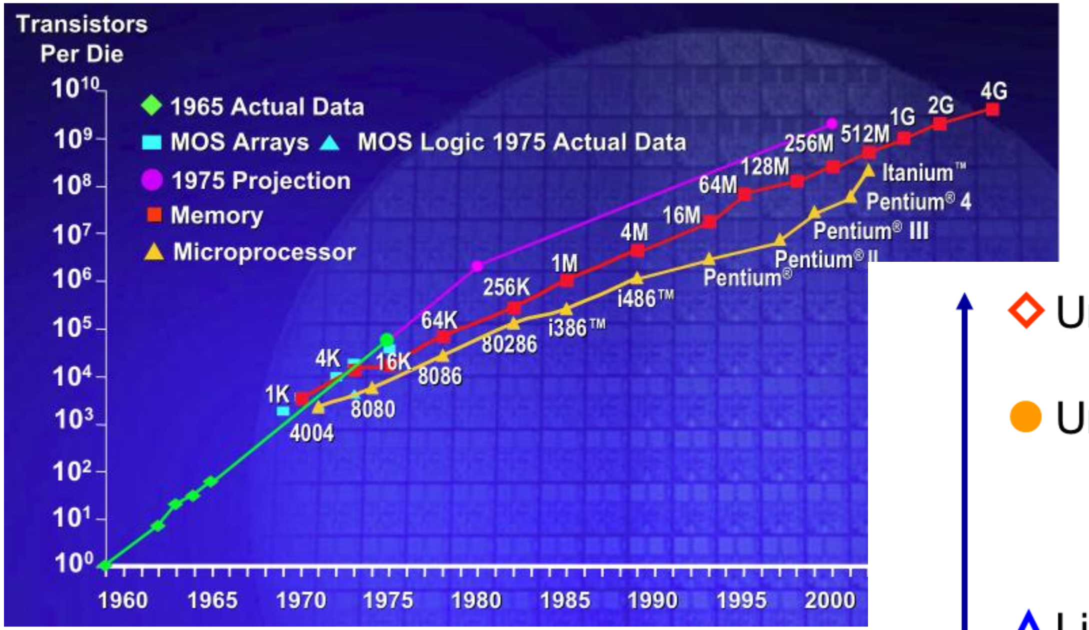
The cathode comprises an Al current collector coated on both sides. The anode comprises a Cu current collector coated on both sides.



Cathode **Separator** **Anode**

Photo image of an 18650 cell

The consequence of understanding is prediction: Moore’s Law for Si *vs*. current strategy for Li-ion batteries



Transformational technologies depend on reliable understanding and control of materials at scales ranging from the atomic to the mesoscale

◇ Unk-HV-HC / Li metal

Safe and reversible cycling of Li metal
Market entry >2021

● Unk-HV-HC / Gr-Si

Discovery of high voltage electrolyte >4.8 V
Discovery of reversible unknown high-voltage high-capacity cathode: 250 mAh/g @ 4.8 V
Market entry > 2019

△ Li_2MXO_4 / Gr-Si

Discovery of path to reversible multi-electron cathode material with 4V cell voltage
Market entry > 2017

■ LMR-NMC / Gr-Si

Stabilization of silicon
Market entry > 2015

◇ LMR-NMC / Gr

Stabilization of LMR-NMC
Market entry > 2013

● LMO / Gr

Nanoscience by the ton

We need a road map for materials development that enables us to escape primitive technologies and have a predictable path forward – this is the science challenge of the next few decades

“Top –down” engineering is not the solution - for example:

- 2/3 of the weight of a PHEV battery is “packaging” – control electronics, safety engineering, casing etc.
- Most of the cost of solar panel installation is *not* the module – power electronics and packaging, installation costs, etc.

Can we learn how to construct functional materials whose properties are defined by precisely controlled interfaces on the nanoscale and which may be manufactured at low cost in enormous volume ....

Breakthroughs Will Rely on New Methodologies

- ***Innovative theory and modeling strategies*** that will span from 'white boards' to exascale computing
- ***New synthetic frameworks*** to discover and grow targeted materials classes
- ***New manufacturing strategies*** utilising self-assembly
- ***In situ tools*** to characterize, understand and control materials growth and function

"Where to put the atoms,
and how to put them there"

Materials by design: genomics?

Genomics must be grounded in theory: the human genome initiative depends fundamentally on the “central dogma” of DNA coding. This is both the fundamental **theory** of biology and an **algorithm**

Materials genomics derives its validity from the Schrodinger equation – but this is not (yet) an instruction set

The Theory of Everything

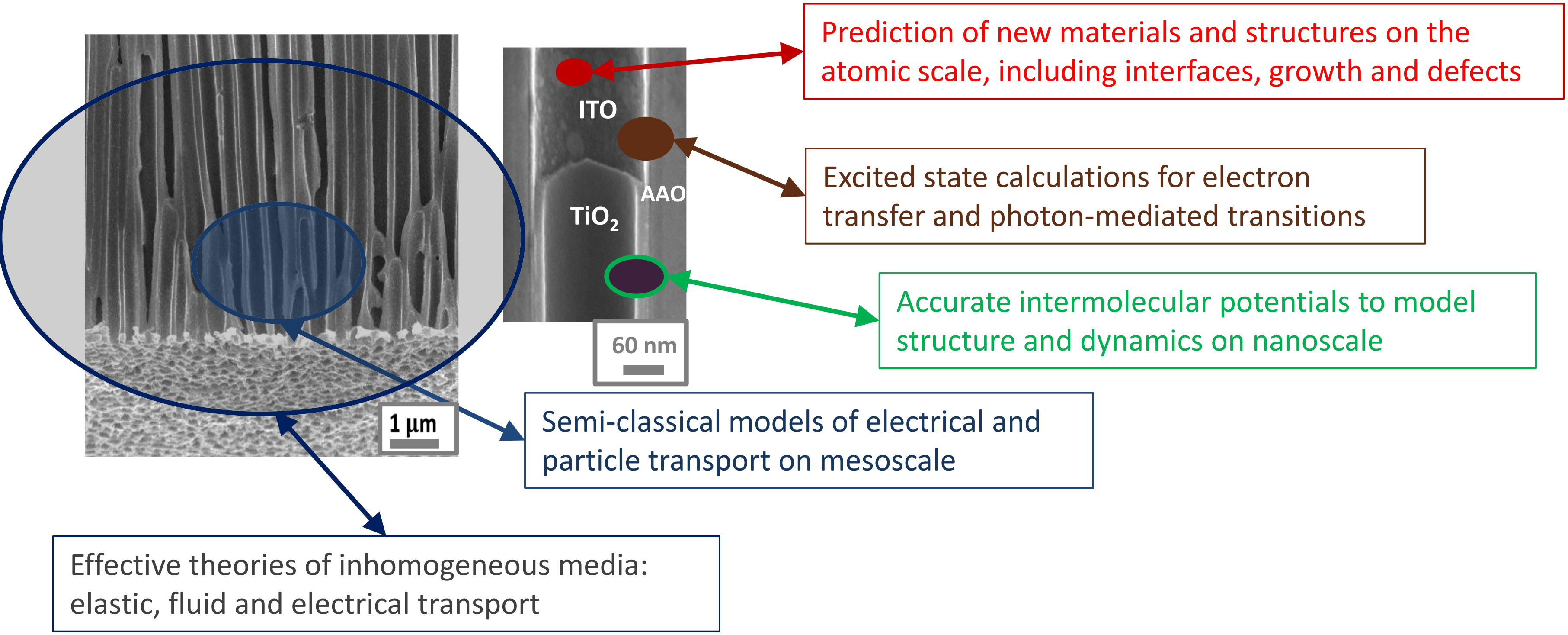
$$i\hbar \frac{\partial \Psi}{\partial t} = \mathcal{H}\Psi$$

$$\mathcal{H} = -\sum_{j}^{N_e} \frac{\hbar^2}{2m}\nabla_j^2 - \sum_{\alpha}^{N_i} \frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 - \sum_{j}^{N_e}\sum_{\alpha}^{N_i} \frac{Z_\alpha e^2}{|\vec{r}_j - \vec{R}_\alpha|} + \sum_{j<k}^{N_e} \frac{e^2}{|\vec{r}_j - \vec{r}_k|} + \sum_{\alpha<\beta}^{N_i} \frac{Z_\alpha Z_\beta e^2}{|\vec{R}_\alpha - \vec{R}_\beta|}$$

- Air
- Water
- Fire
- Rocks
- Cement
- Steel
- Plastic
- Glass
- Wood
- Asphalt
- Paper
- Dynamite
- Antifreeze
- Glue
- Dyes
- Vitamins
- Ham Sandwiches
- Ebola Virus
- Economists
- ...

Robert Laughlin (Nobel lecture)

Computational Chemistry and Materials Science: designing what you make



Prediction of new materials and structures on the atomic scale, including interfaces, growth and defects

Excited state calculations for electron transfer and photon-mediated transitions

Accurate intermolecular potentials to model structure and dynamics on nanoscale

Semi-classical models of electrical and particle transport on mesoscale

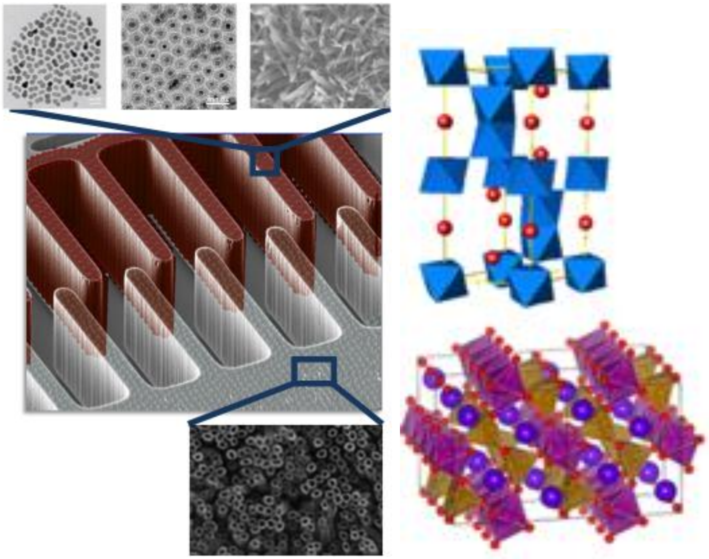
Effective theories of inhomogeneous media: elastic, fluid and electrical transport

- Each box requires new investment in methods, theory and computation
- Joining up the boxes is as important as the investment in any single piece
- We must curate both data and software
- Design choices driven by application target

Demands a collective corporate effort linking computation, methods, software, and data guided by an engineering goal

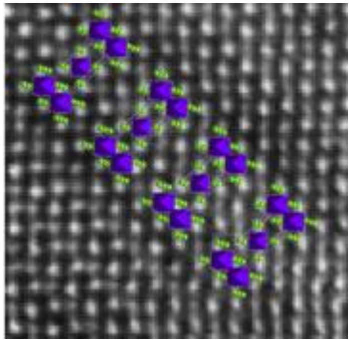
From synthesis to manufacturing: Can you actually make what you have designed?

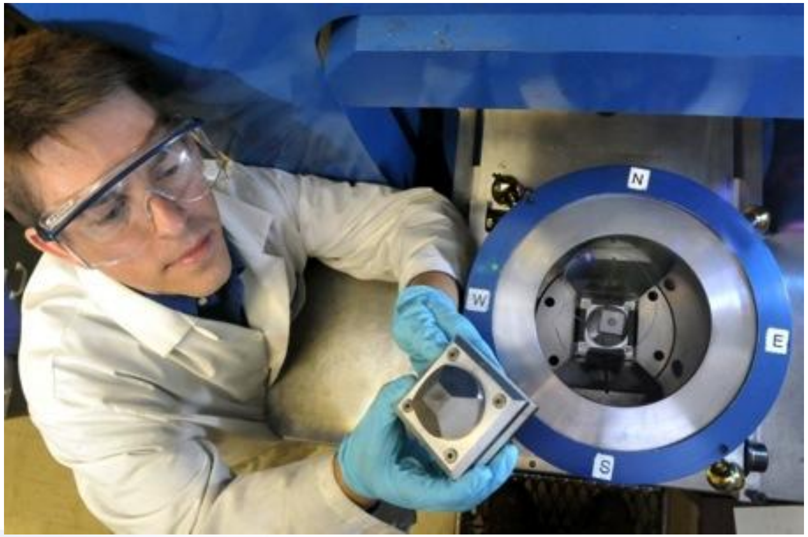
Goal: Create completely new classes of materials by coordinating the science of synthesis with the science of function.



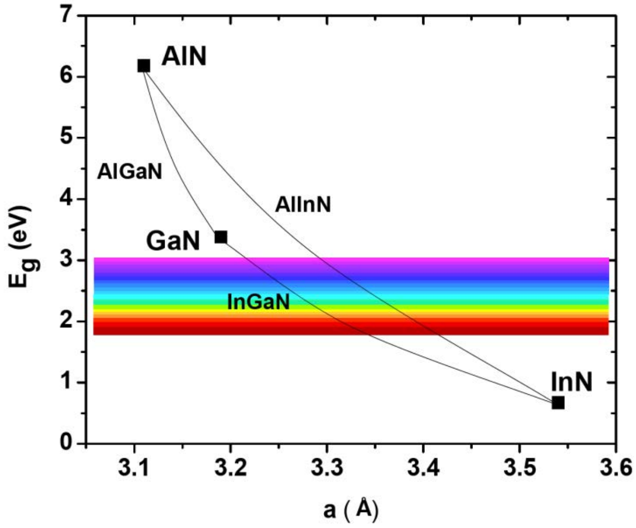
Approach:

- Materials design and synthesis
- Control and characterization using *in situ* monitoring of processing
- Accelerated materials discovery *via* high throughput computational design and modeling

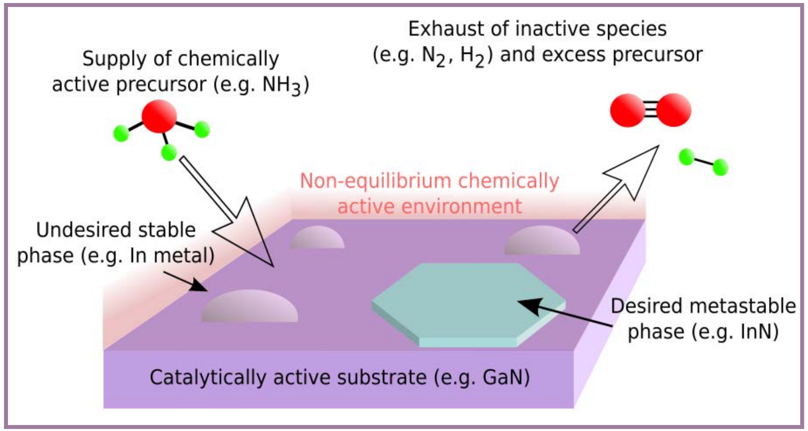




The green LED problem: control of vapor phase growth



Materials Synthesis



Supply of chemically active precursor (e.g. NH_3)

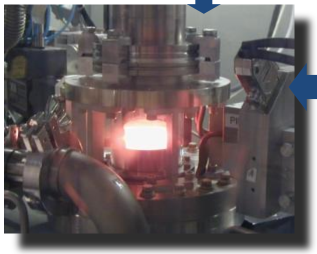
Exhaust of inactive species (e.g. N_2, H_2) and excess precursor

Non-equilibrium chemically active environment

Undesired stable phase (e.g. In metal)

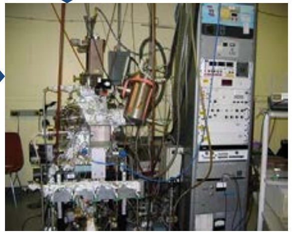
Desired metastable phase (e.g. InN)

Catalytically active substrate (e.g. GaN)



In situ X-ray

Theory and Modeling



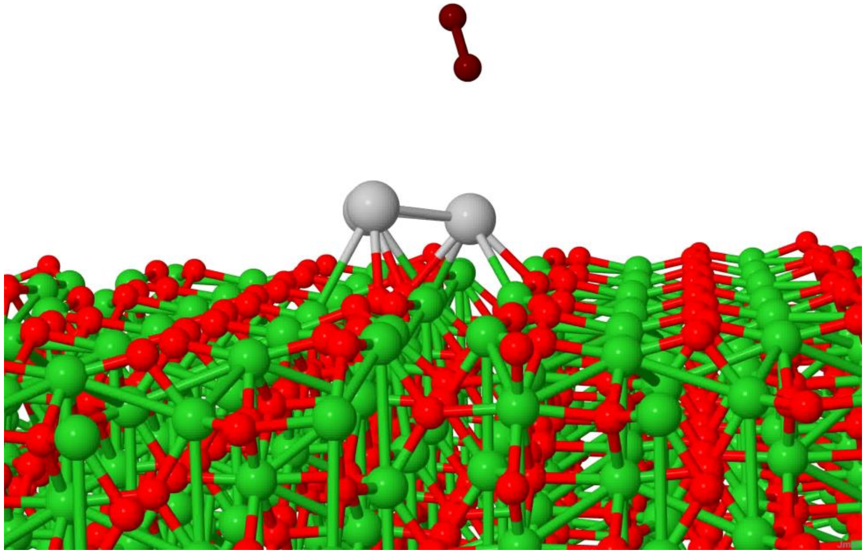
In situ Infrared Spectroscopy

Develop an integrated computational model of (In,Al)N growth using LCF, validate by *in situ* probe at APS

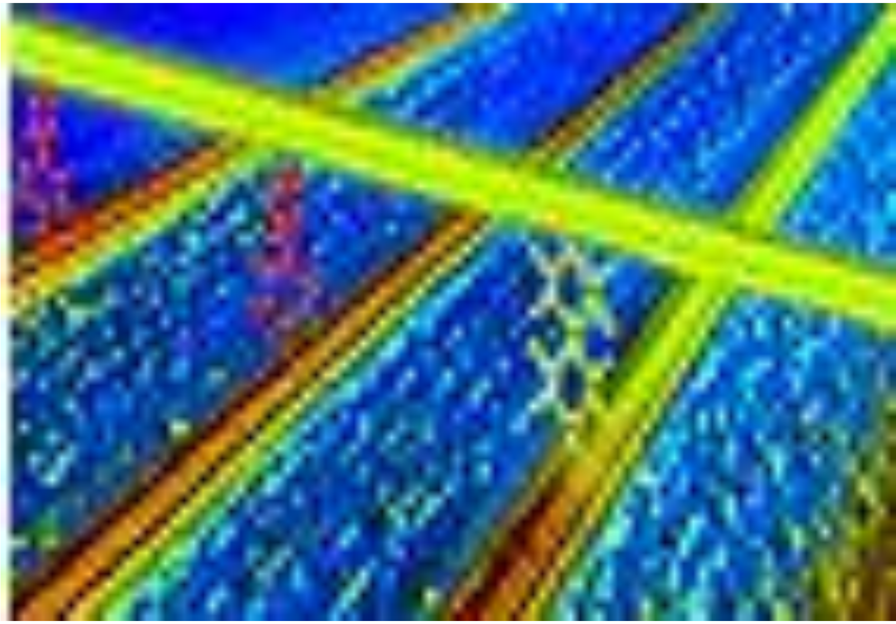
Design of catalysts: direct oxidation of propylene

- Major industrial process, no known direct route
- Sub-nm Ag_3 most active reported to date
- Size-selected cluster deposition from molecular beams
- In situ X-ray scattering and X-ray photoelectron spectroscopy combined with temperature-programmed reactivity
- State of the art modeling

Publication in Science in 2010
2 US patents in 2012
Negotiating licensing

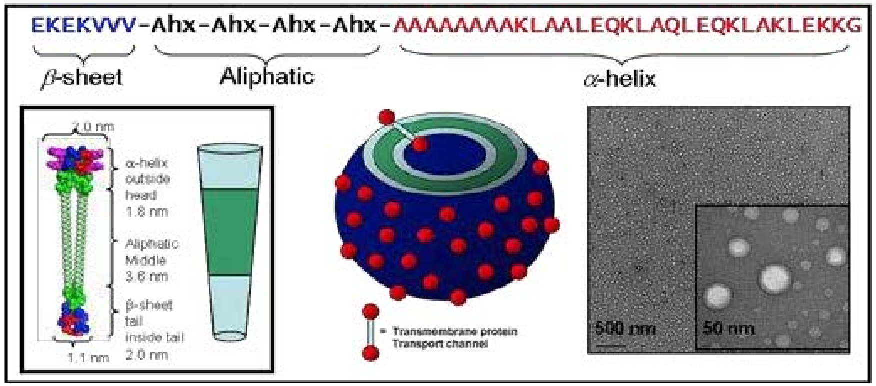


Institute for Molecular Engineering: Partnership between University of Chicago and Argonne

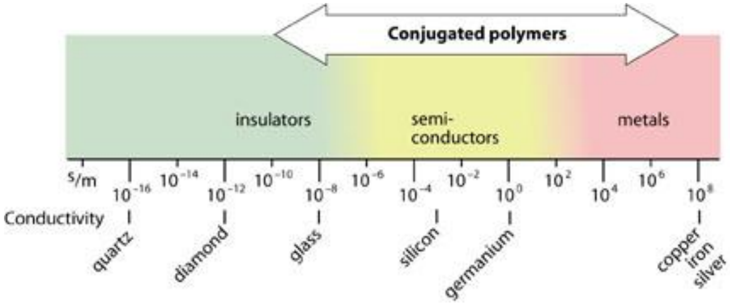


- Science is about discovery, engineering is about invention; they are mutually complementary, deeply creative activities
- A motivating idea of Molecular Engineering is to exploit molecular-level science to develop solutions to societal problems in
  - Energy
  - Information technology and communications
  - Environment and sustainability
  - Healthcare
- These areas of importance are not distinct from one another

Build teams of enabling technologies … not traditional engineering departments



- Materials science
  - Synthesis, organic, inorganic and processing
- Catalysis and reactive materials
- Biological engineering
  - Synthetic biology, bio-inspired and bio-derived materials
- Imaging and structure determination in real and reciprocal space
- Functional assemblies
  - Electronic, photonic, micromechanical/ robotic and membranes
- Computational engineering and predictive modeling



Materials for Energy: Argonne’s Vision

Materials science, chemistry and modeling for transformational change in energy technologies

- Goal: Accelerate materials discovery, design and manufacturing - from atomic through mesoscale

  … which enables an energy strategy for the nation

  … and encourages stable investment in next generation technologies

- Foundation: Argonne’s (and partners’) strengths
  - Facilities: APS, ALCF, CNM, EMC
  - Staff: Strong PI-driven science programs in MSD, CSE, CNM, MCS
  - Universities: UChicago, Northwestern, UIC, UIUC, ...
  - Partnerships: EFRCs, other DOE labs, industry
  - Environment: Technology handshake with energy applications: e.g. in storage, solar, refrigeration, transmission, lighting, combustion, catalysis and generation

Materials for energy: Argonne's strategy

Partnerships with local universities and with global industry to build critical mass in foundational problems – regional "hubs"

- Computational chemistry and materials science
- Science of Synthesis
- Institute of Molecular Engineering