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Multiscale Materials Modeling At the University of Tennessee

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Scholars Invitational
University of Tennessee, Knoxville
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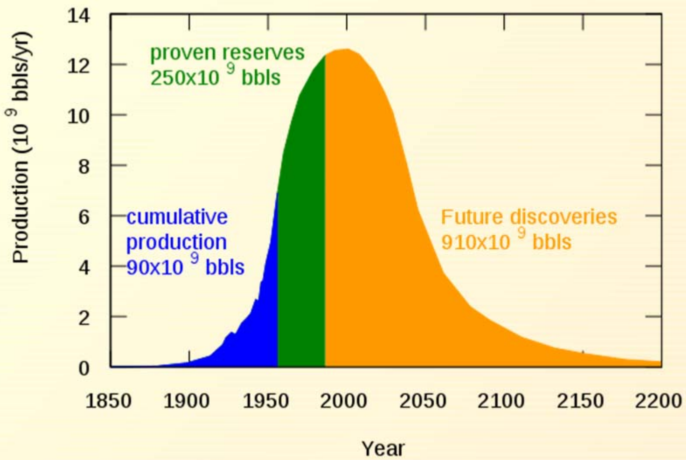
Multiscale Materials Modeler

Renewable Energy: The Defining Challenge of Your Generation



Peak Oil

Fossil fuels are a finite resource

http://en.wikipedia.org/wiki/Peak_oil

Climate Change

Atmospheric CO_2 over the past 1100 years

Sustainability without the Hot Air, MacKay

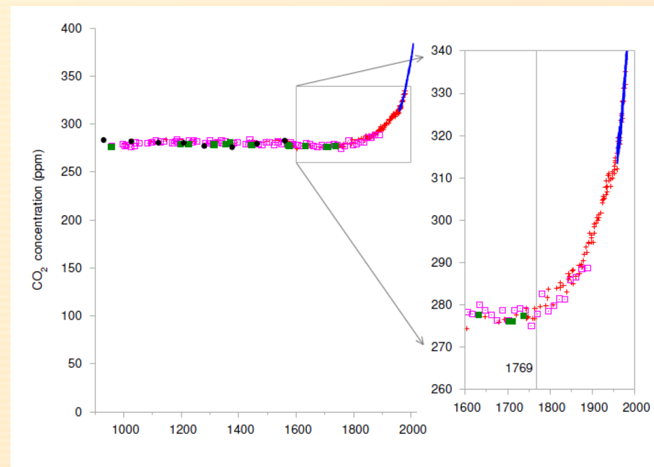
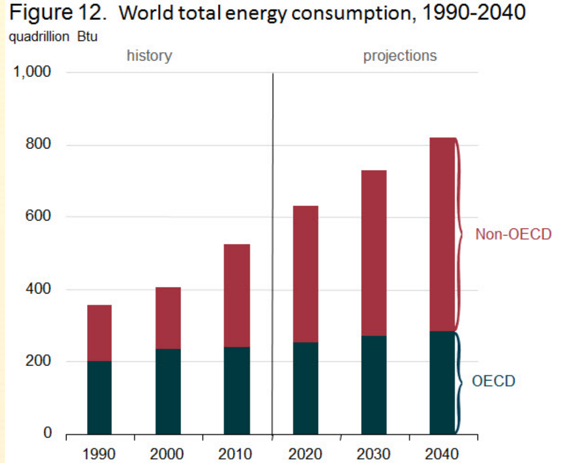


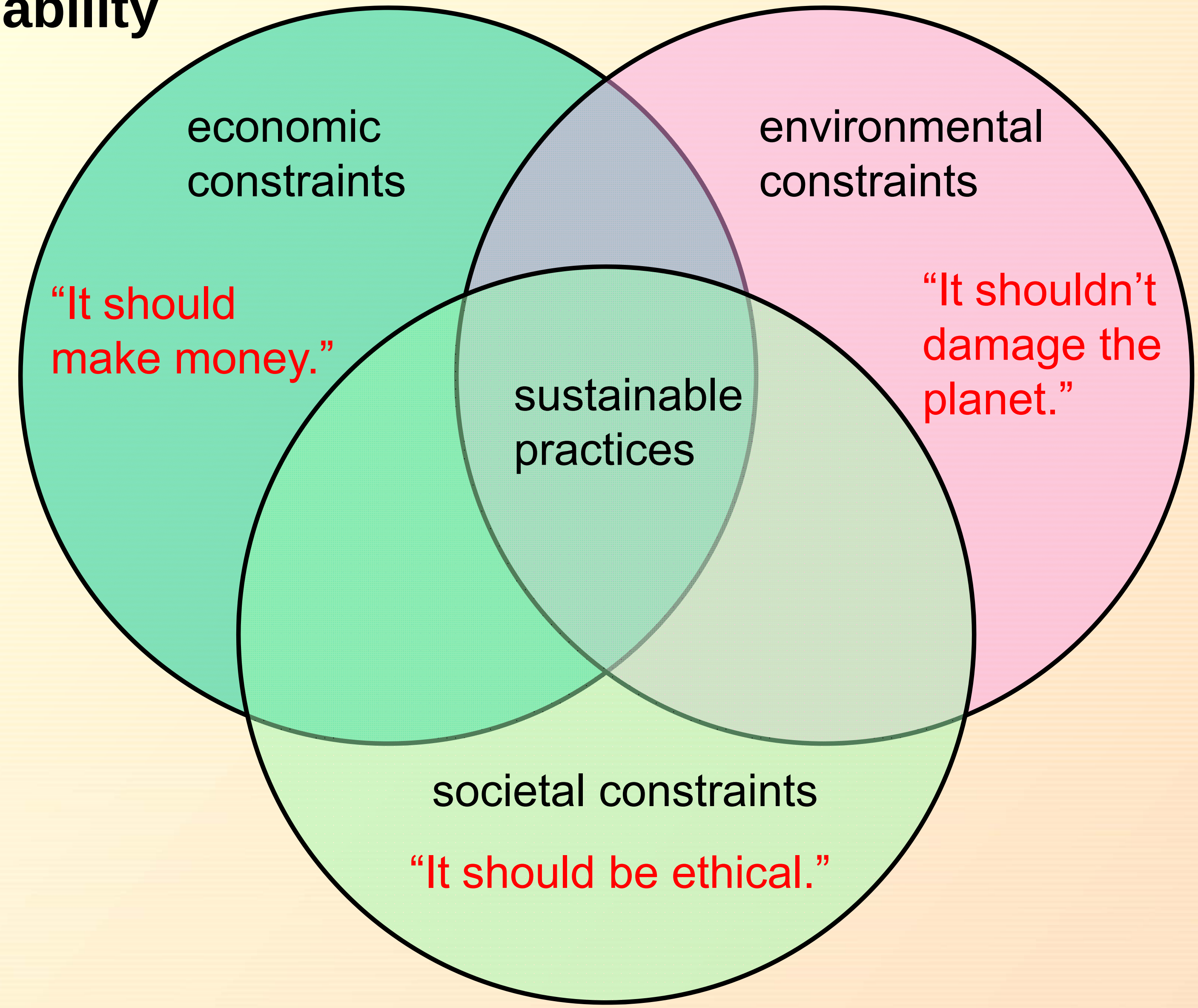
Figure 12. World total energy consumption, 1990-2040



Global Energy Demand is Rising

http://www.eia.gov/forecasts/ieo/world.cfm

Sustainability



Interdisciplinary problem: Materials Scientists play critical role.

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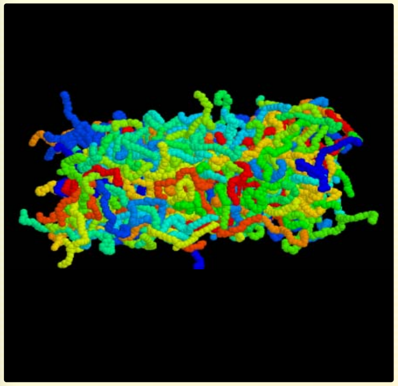
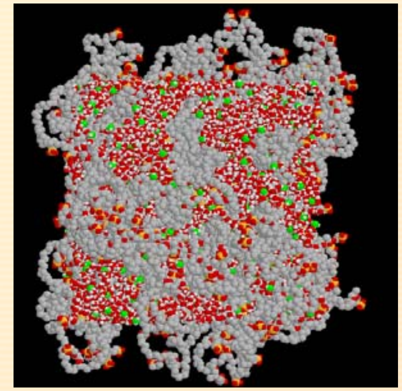
Apply simulation tools to develop structure/property relationships

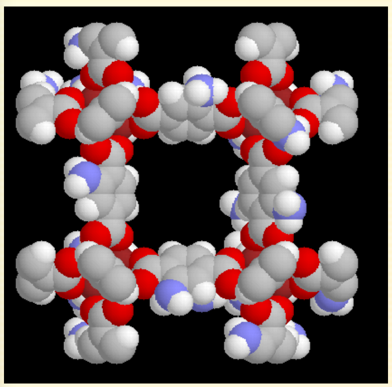


polymeric materials

polymers at equilibrium and under flow (PE, PET)

polymer electrolyte membranes (PEMs) in fuel cells

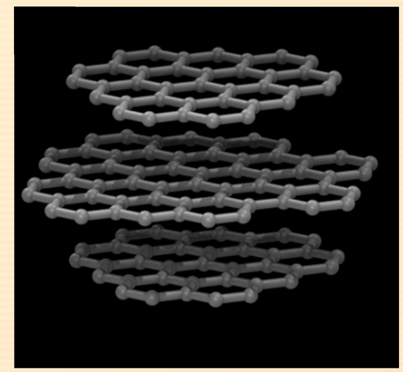


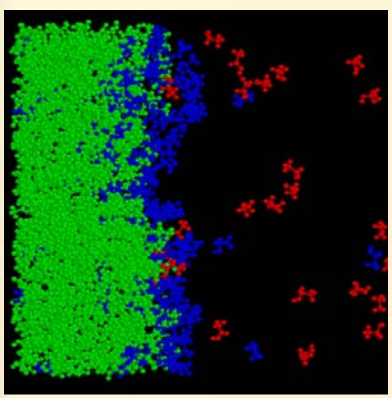


nanoporous materials

hydrogen sorption in metal organic frameworks (MOFs)

bio-derived, nanostructured battery anodes

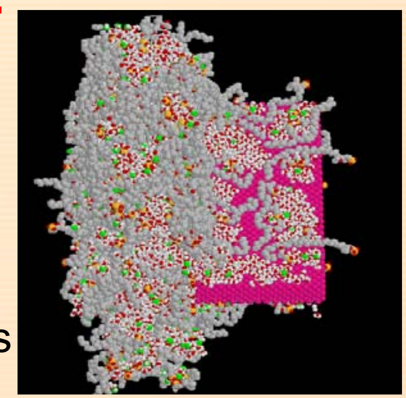




interfacial systems

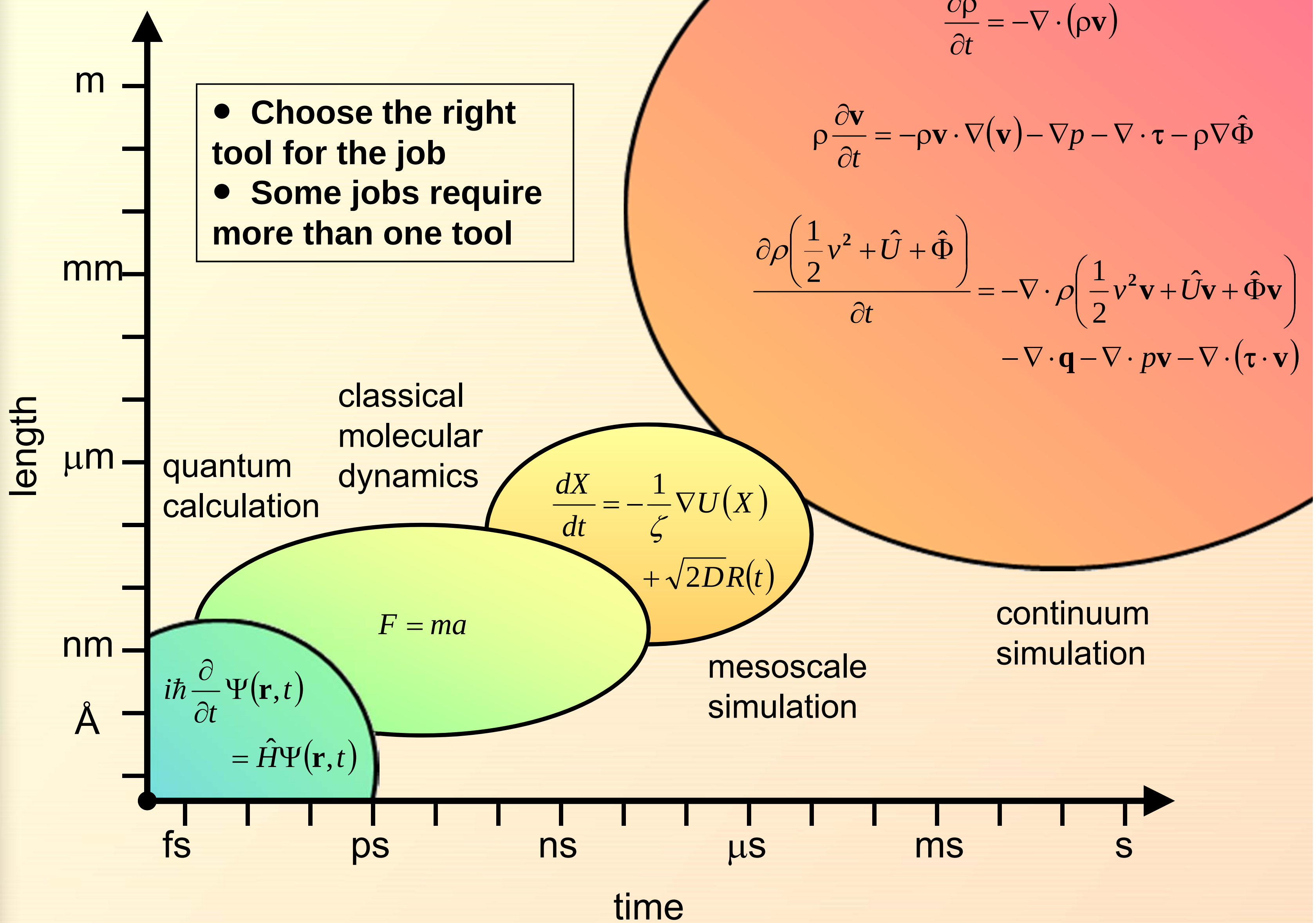
near critical vapor-liquid interface structure

fuel cell electrode/ electrolyte interfaces



Time and Length Scales

- Choose the right tool for the job
- Some jobs require more than one tool



Collaboration with Oak Ridge National Laboratory

OAK RIDGE NATIONAL LABORATORY

Managed by UT-Battelle for the Department of Energy

National Center for Computational Science

Today the computing resources of the NCCS are among the fastest in the world, able to perform more than 119 trillion calculations per second.

To solve systems of ODEs (largest system thus far is several million), we use the massively parallel supercomputers at ORNL.

These resources are available to researchers at UT through discretionary accounts of the program directors.

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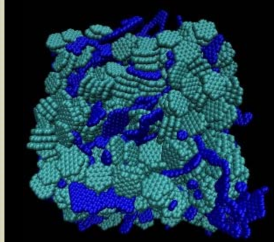
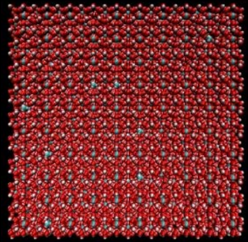
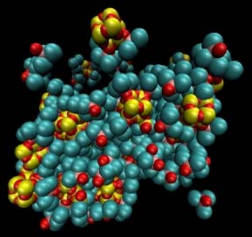
A Complementary Tool: Experimental Collaborators (2013)



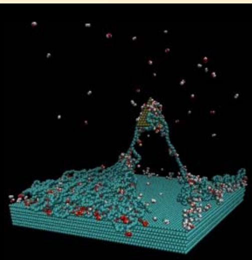
Orlando Rios
(ORNL)
nanostructured
battery
electrodes



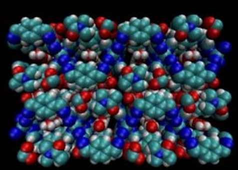
Claudia Rawn
(UT MSE)
methane &
carbon dioxide
hydrates



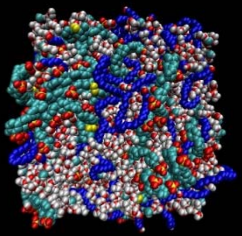
Craig Barnes
(UT Chem)
nanostructured
single-site
catalysts



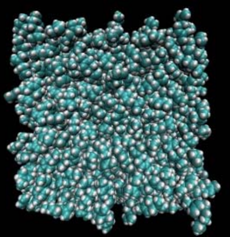
David Joy
(UT MSE/ORNL)
PEM fuel cell
catalyst layer



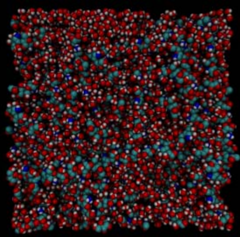
David Jenkins
(UT Chem)
breathable
metal-organic
nanotubes



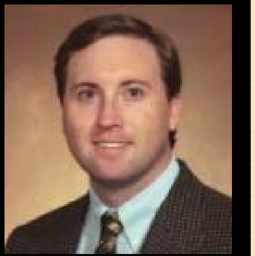
Jimmy Mays
(UT Chem/ORNL)
fuel cell
proton exchange
membranes



Bob Compton
(UT Phys)
racemic
mixtures



Kevin Kit
(UT MSE)
renewable
polymer
films

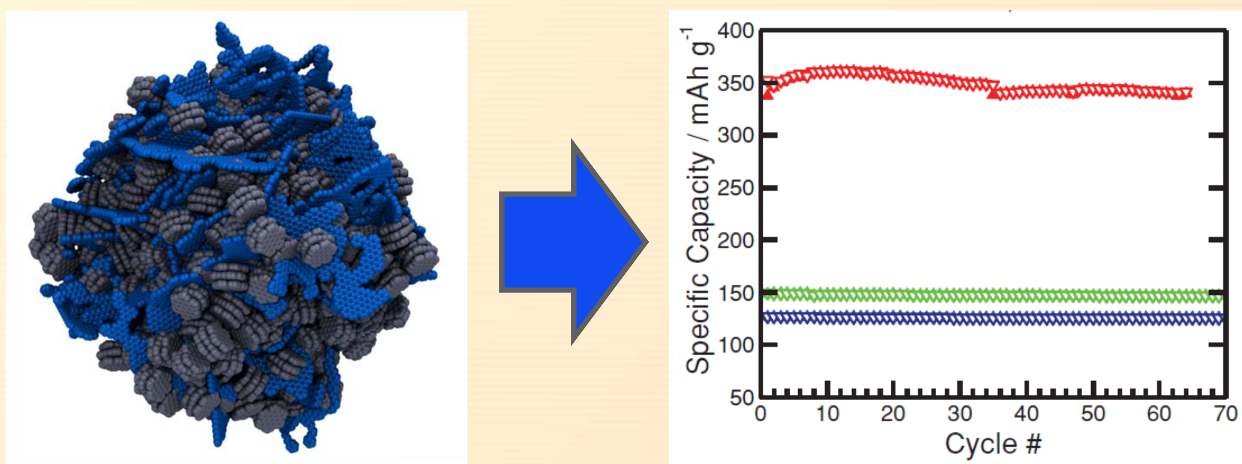


Multiscale Modeling of Carbon Composite Electrodes From Renewable Materials

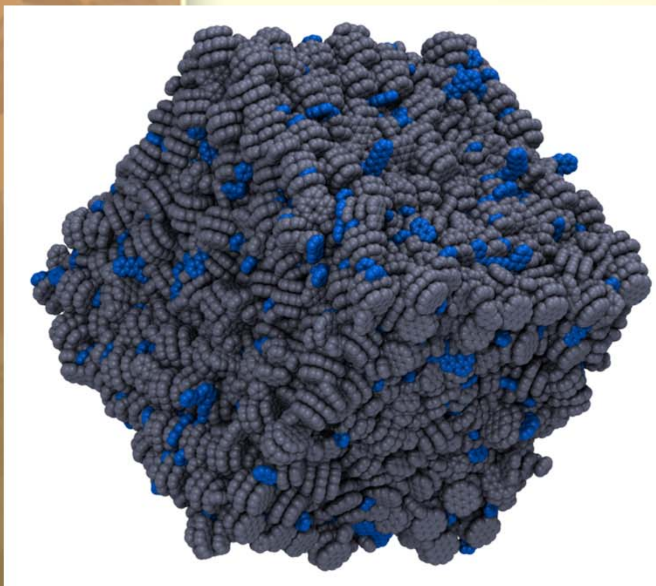
David J. Keffer[1], Nicholas W. McNutt, Khorgolkhuu Odbadrakh & Orlando Rios[2]
[1]University of Tennessee & [2]Oak Ridge National Laboratory

dkeffer@utk.edu

Objective: The objective of this work is to understand the molecular-level mechanisms responsible for the exceptionally high ion storage and fast charging and discharging rates observed in the novel lignin-based carbon composite electrodes synthesized by Rios at ORNL. This knowledge can be used to further guide development of improved materials for battery electrode applications.



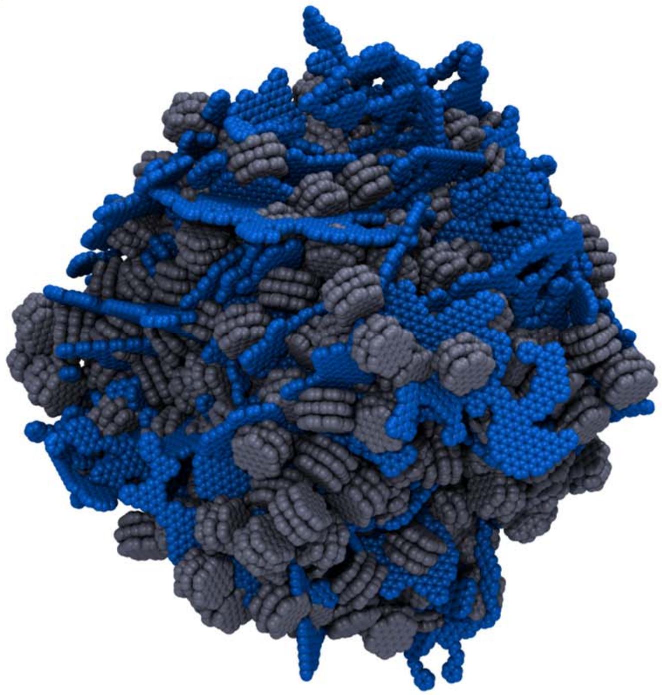
Molecular Models of Experimentally Synthesized Composites



Pyrolysis temperature controls nanostructure.

1500 K		
r_c	=	7 Å
Φ_c	=	0.5
ρ	=	1.51 g/cm^3

1000 K		
r_c	=	5 Å
Φ_c	=	0.9
ρ	=	1.94 g/cm^3

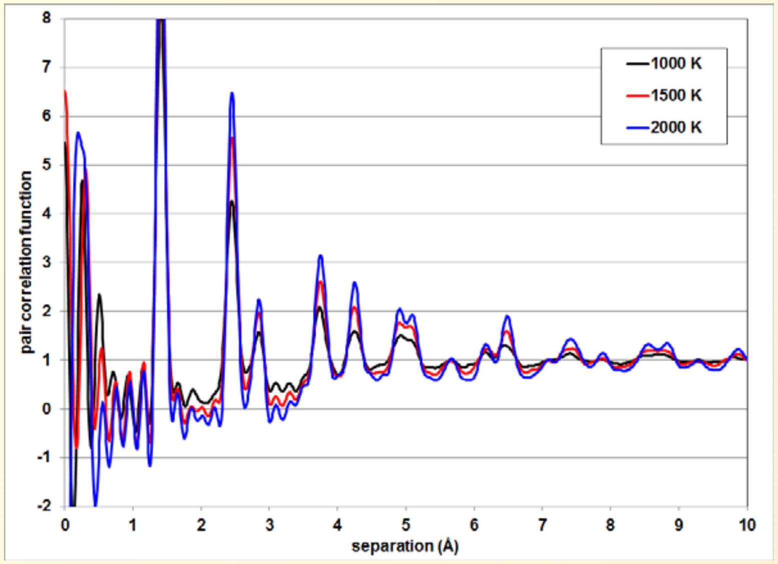


2000 K		
r_c	=	17 Å
Φ_c	=	0.1
ρ	=	1.38 g/cm^3

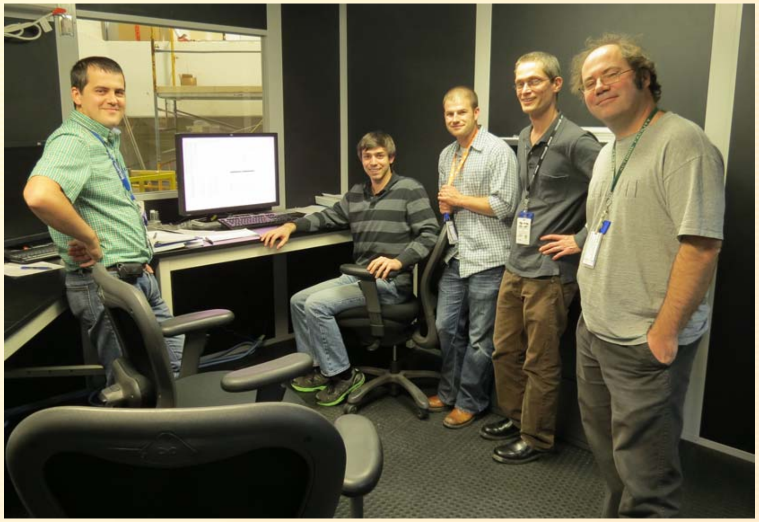
The composite materials are composed of graphitic nanocrystallites (gray) and amorphous carbon (blue).

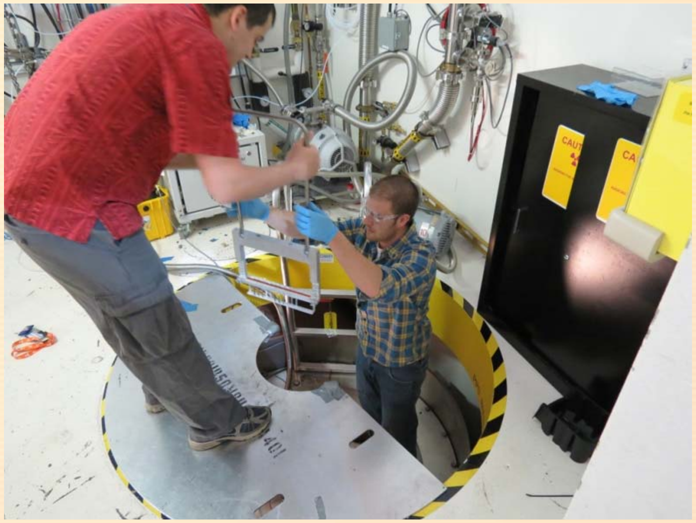
These models capture experimental crystallite size, crystalline volume fraction and total density.

Neutron Diffraction from NOMAD

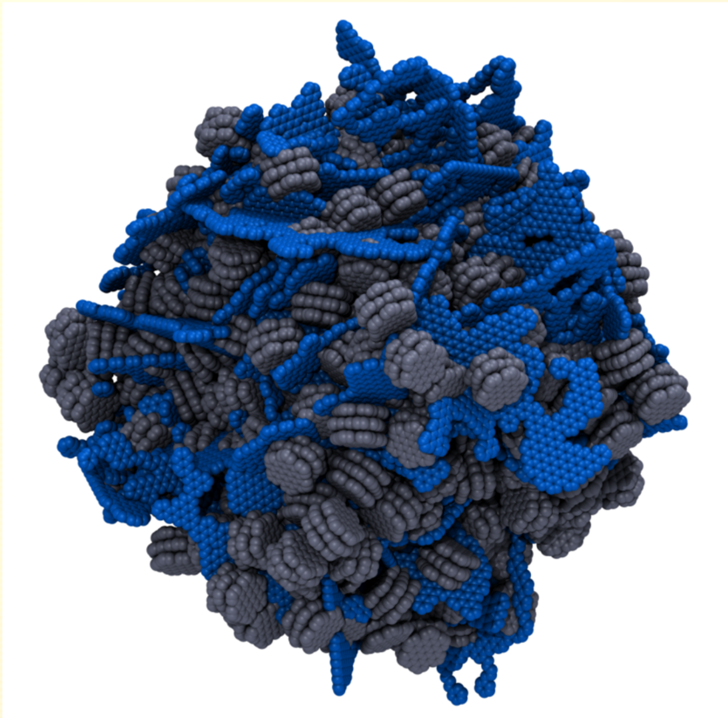


NOMAD is a high-flux, medium-resolution diffractometer that uses a large bandwidth of neutron energies and extensive detector coverage to carry out structural determinations of local order in crystalline and amorphous materials.





Interpretation of Nomad Data



1500 K

r_c	=	7 Å
Φ_c	=	0.5
ρ	=	1.51 g/cm^3

Process

Modelers use their knowledge and imagination to hypothesize structures.

Perform MD simulations.

Generate pair correlation functions (PCFs).

Compare simulated and experimental PCFs.

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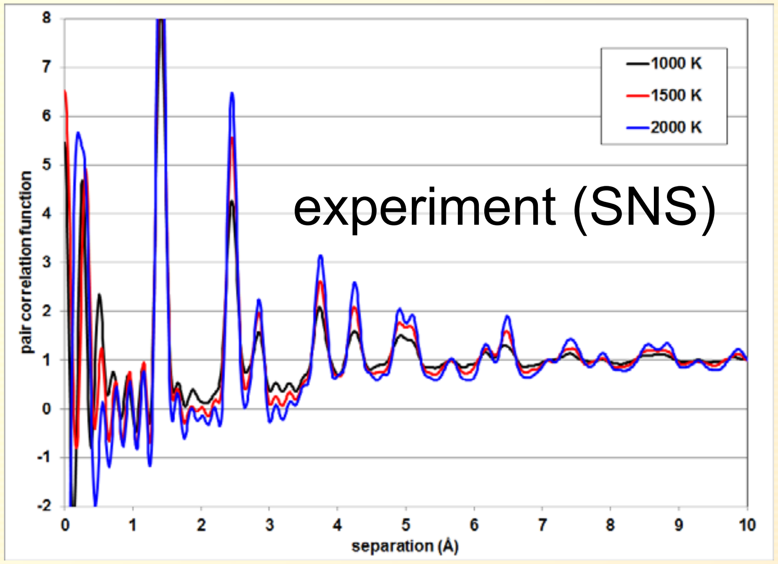
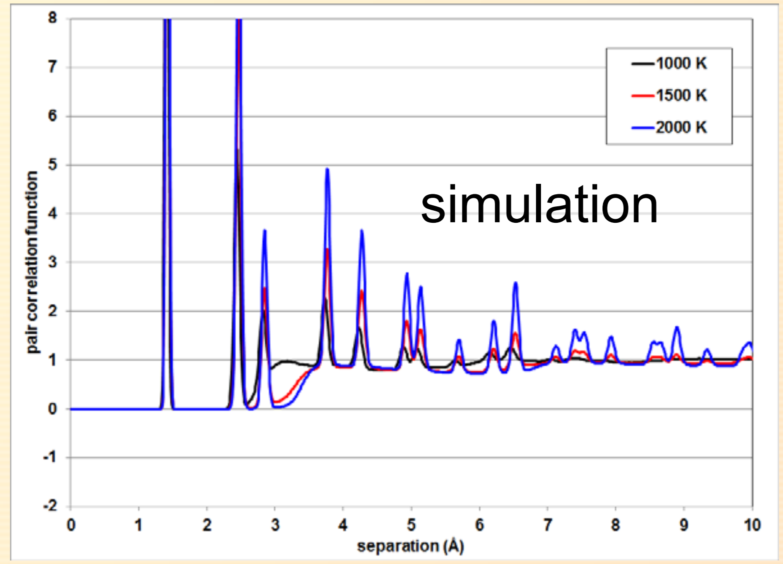
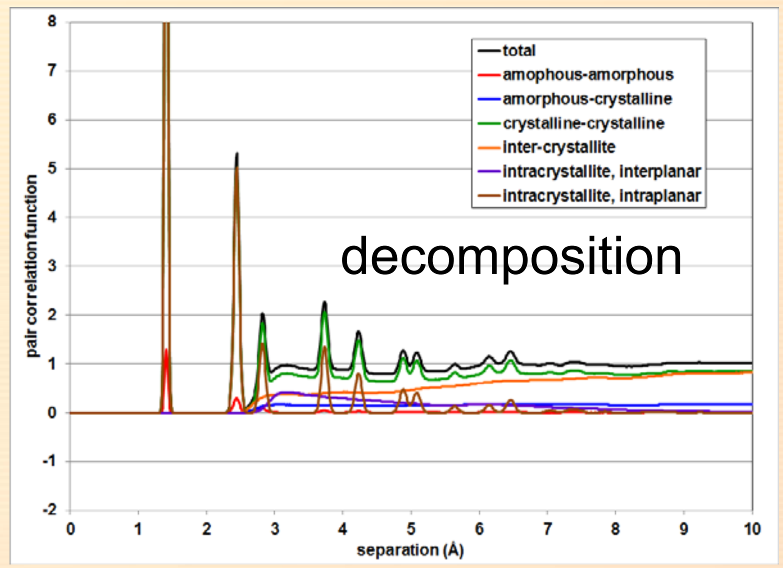
Composite Models Provide Interpretation of Neutron Data

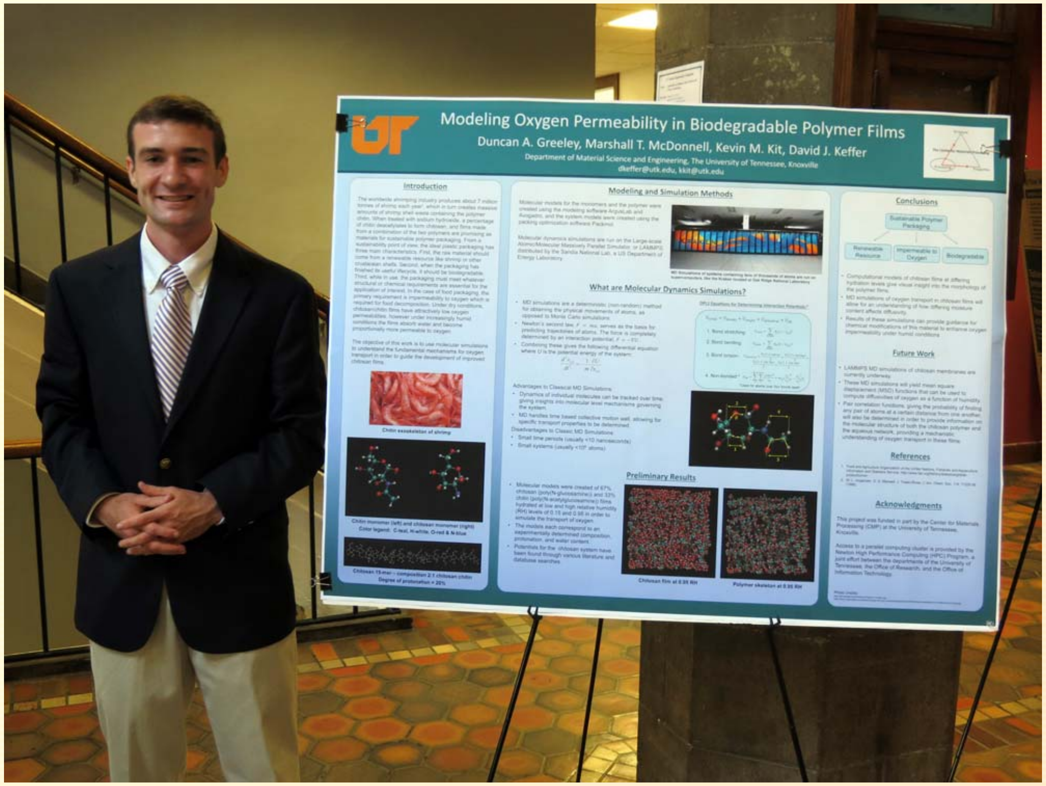


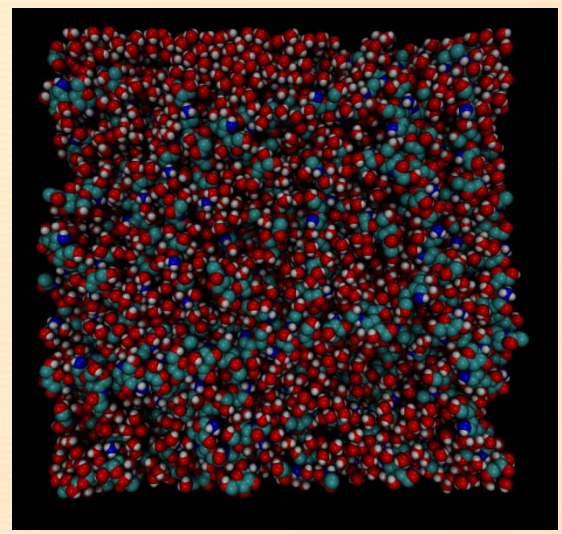


Neutron diffraction data from the SNS (top left) are difficult to interpret for even partially amorphous materials. However, clear trends are seen with respect to pyrolysis temperature. Pair correlation functions (PCFs) for the corresponding models (top right) provide clean, unambiguous data. Moreover, the simulated PCFs can be completely decomposed (right) to reveal the structural origins of all features in the spectra, providing clear understanding of the experimental data from the SNS.



Undergraduates Perform Research in MSE at UT





Duncan Greeley performs MD simulations of oxygen transport in chitosan films to provide insight into biodegradable plastics made from renewable resources. (2013)

Conclusions

- The search for renewable energy sources and systems is the defining challenge of your generation.
- Materials Scientists & Engineers play a critical role in this search for sustainability.
- Students in the Materials Science & Engineering Department at the University of Tennessee are performing state-of-the-art research using the world's best supercomputers and neutron sources to develop new materials for alternative energy systems.
- Multiscale Materials Modeling is a complementary tool to experiment, providing unique insight.
- Experimental/Computational collaborations are fruitful and fun!

UT Materials Structure Interactive Gallery

http://utmsig.utk.edu/

This site features interactive structures from various materials research projects (both computational and experimental) performed in the Department of Materials Science and Engineering at the University of Tennessee.

Questions?