Argonne National Laboratory: Innovative Research in the National Interest

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Argonne Training Program on Extreme-Scale Computing
Pheasant Run Resort
St. Charles, IL
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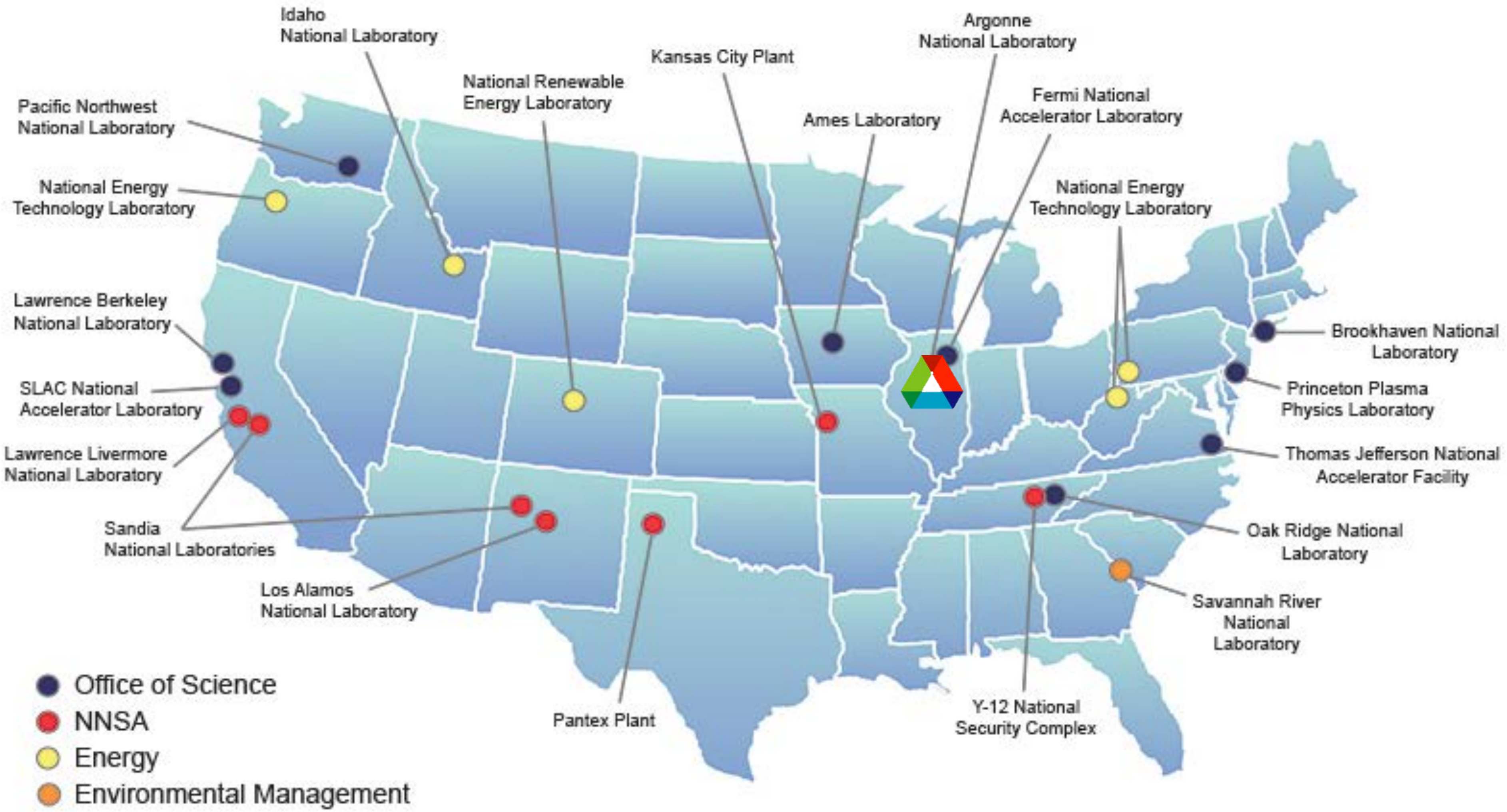
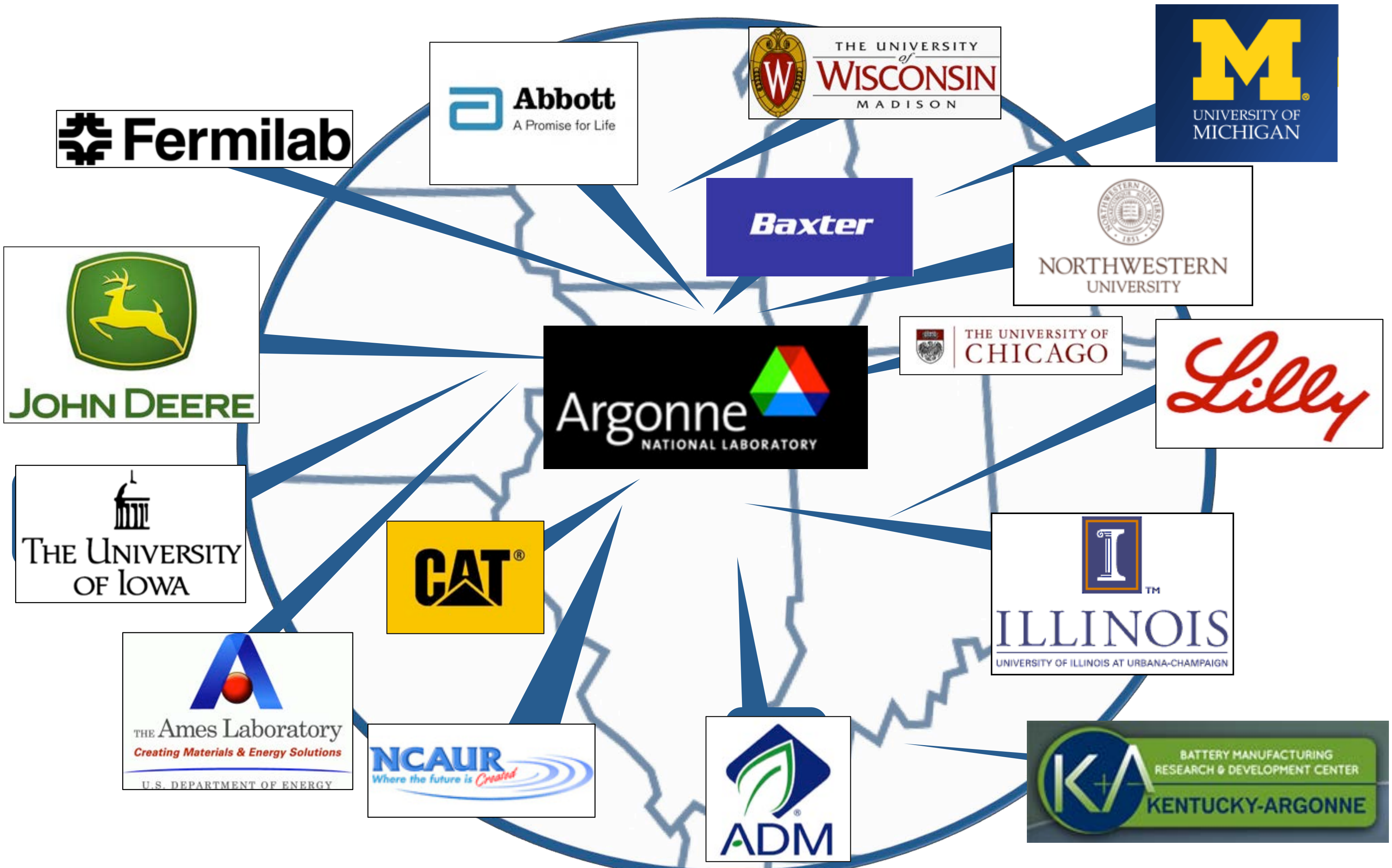
Argonne National Laboratory

Argonne integrates world-class science, engineering, and user facilities to deliver innovative research and technologies

Argonne – a vital part of DOE National Laboratory System



Argonne is at the hub of America's innovation heartland



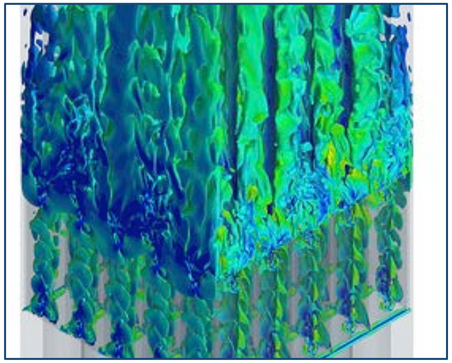
Argonne's mission: Delivering science-based solutions to national energy challenges

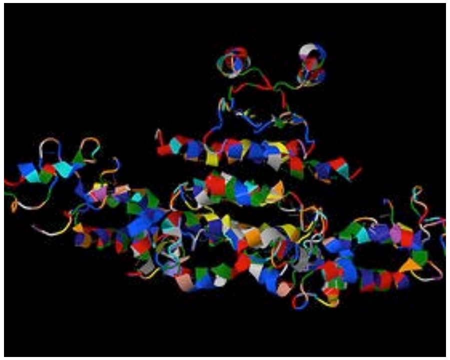
Through discovery and transformational research

World-leading hard x-ray sciences & sources	Discovery science for energy	Leadership computing and computational ecosystem	Fundamental physics and accelerator science	Materials & systems engineering solutions

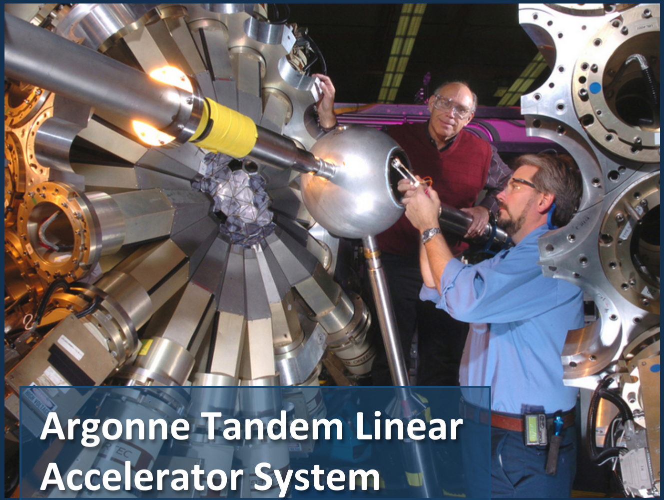
and use-inspired science and engineering

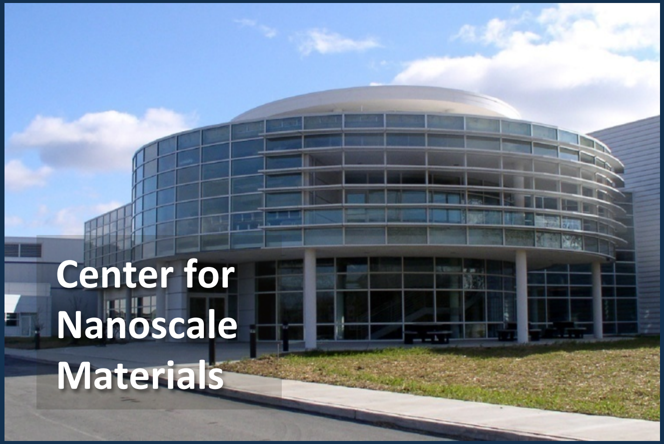
Energy Storage	Sustainable Transportation	Nuclear Energy & Security	Biological & Environmental Systems

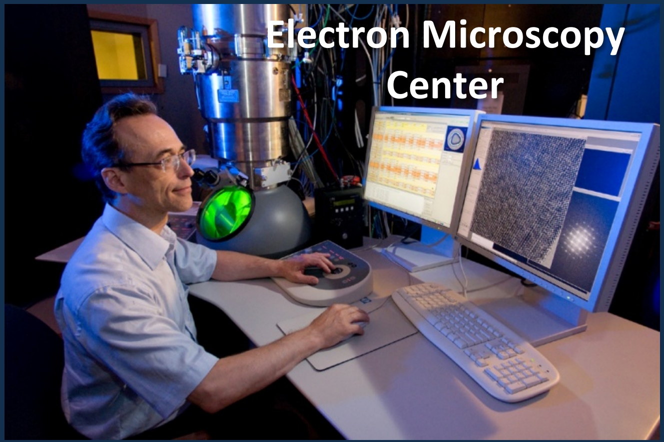




Argonne offers a unique suite of major scientific facilities

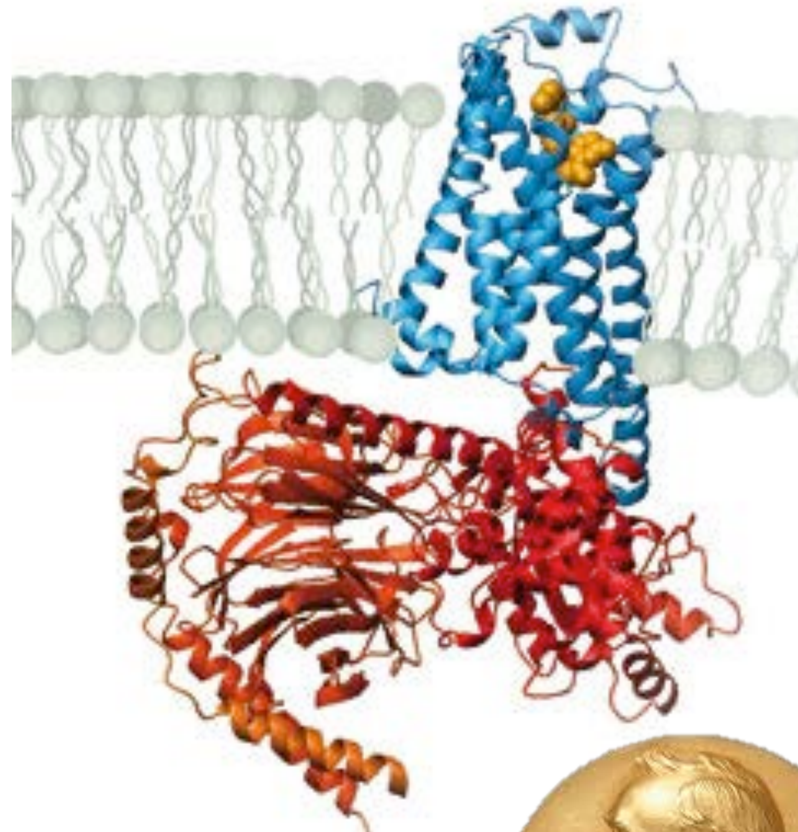






The Advanced Photon Source: The brightest, sharpest x-rays in the Western Hemisphere

- Powerful APS x-ray beams help scientists see things in unprecedented detail, get extraordinary results, extremely quickly
- The APS is a tremendous tool for almost every scientific discipline, from materials science to biology, chemistry, environmental science, and fundamental physics
- Used by >5,000 scientists each year, from private industry, universities, medical schools and research laboratories across the country and around the world



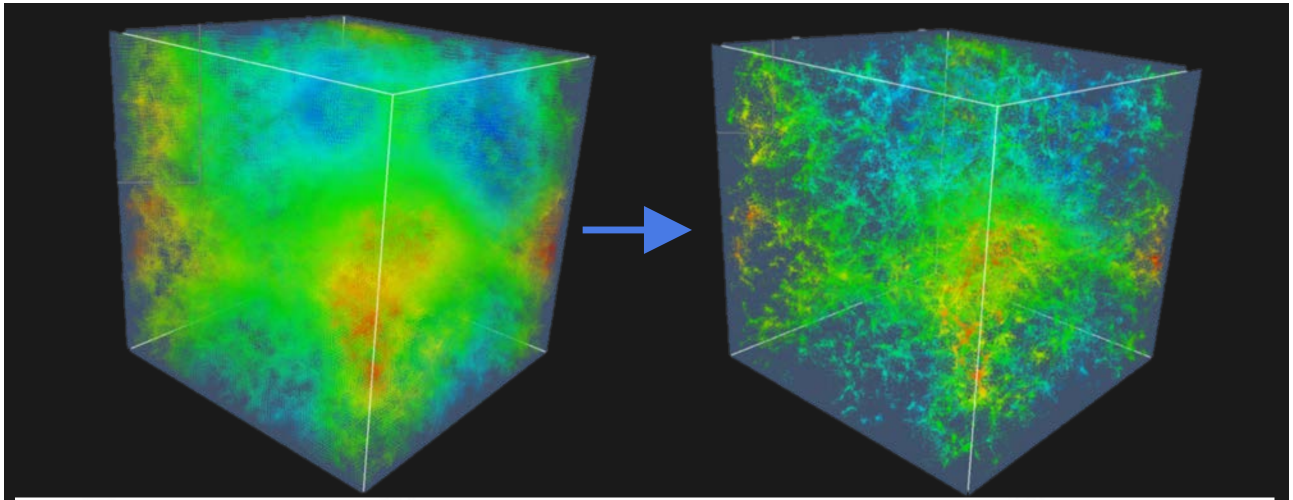
Nobel Prize
in Chemistry
2012

Mira

As scale of national challenges expands, HPC plays increasing role in scientific inquiry

South Pole Telescope

- Scale of leading-edge science yielding very large datasets
- Massively parallel computing necessary for analysis, modeling and simulations
- HPC is key to the future of science (and technology)



$$\nabla^2\phi = 4\pi G a^2(\rho(\mathbf{x},t) - \langle\rho_{\rm dm}(t)\rangle) = 4\pi G a^2\Omega_{\rm dm}\delta_{\rm dm}\rho_{\rm cr},$$

Precision Cosmology, Salman Habib, ANL

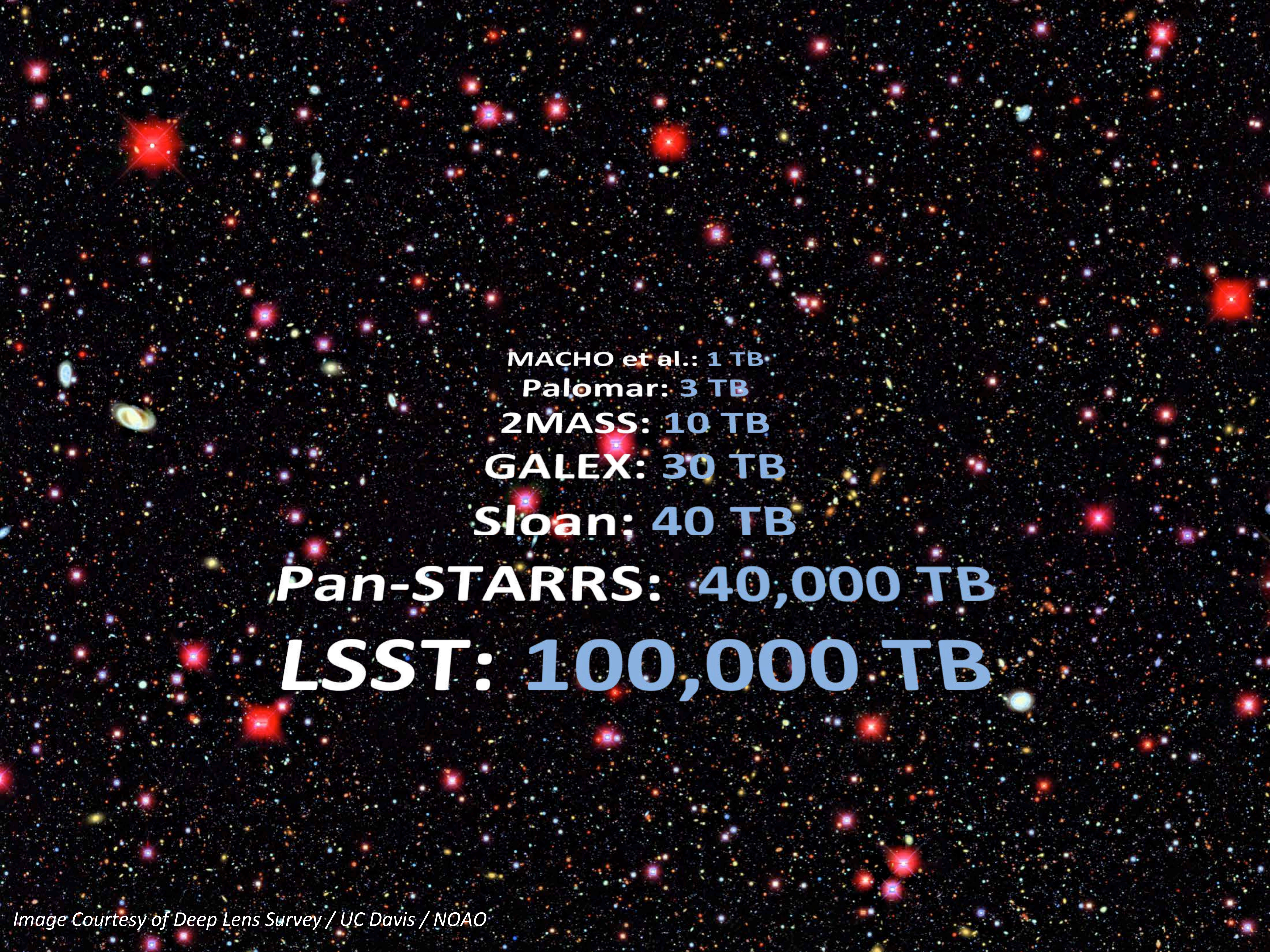
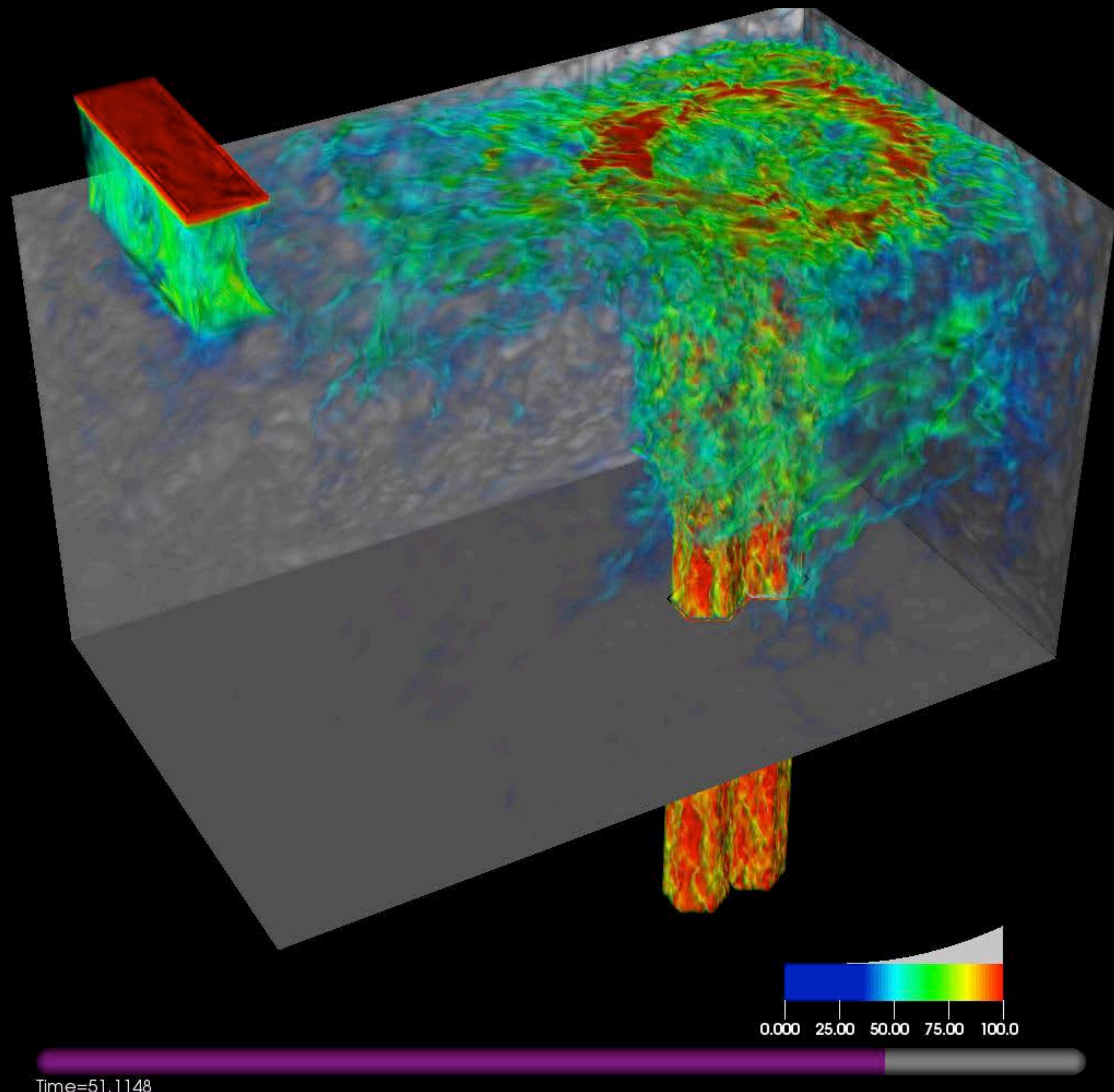


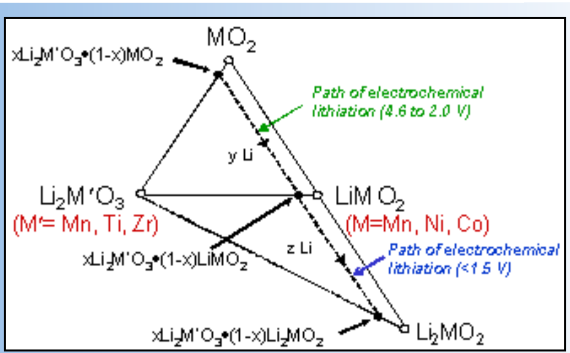
Image Courtesy of Deep Lens Survey / UC Davis / NOAO

Argonne's unique suite of scientific facilities enables cross-disciplinary discovery

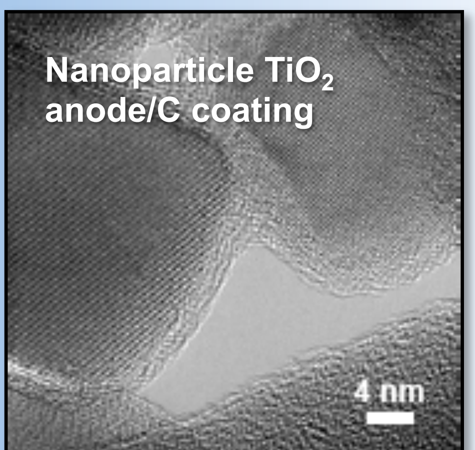
Argonne's major research initiatives bring together `dream teams' to address grand challenges



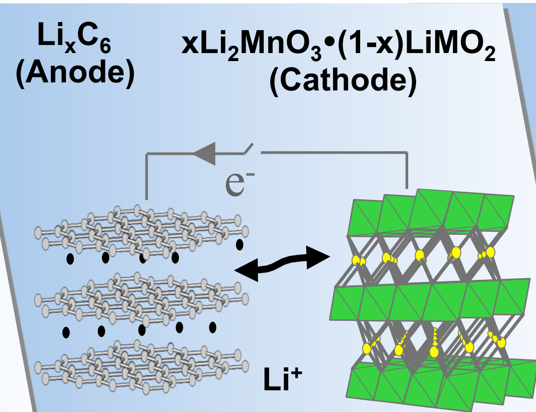
Argonne's battery research program: From fundamental research to cars on the road



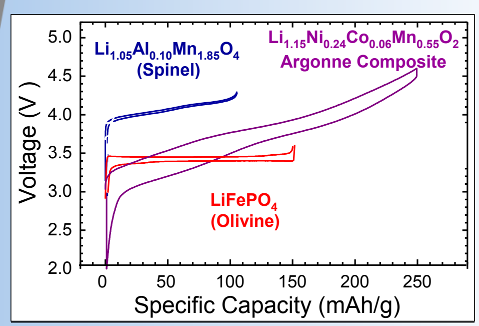
Discovered new composite structures for stable, high-capacity cathodes



Tailored electrode-electrolyte interface using nanotechnology



Created high-energy Li-ion cells with double cathode capacity, enhanced stability

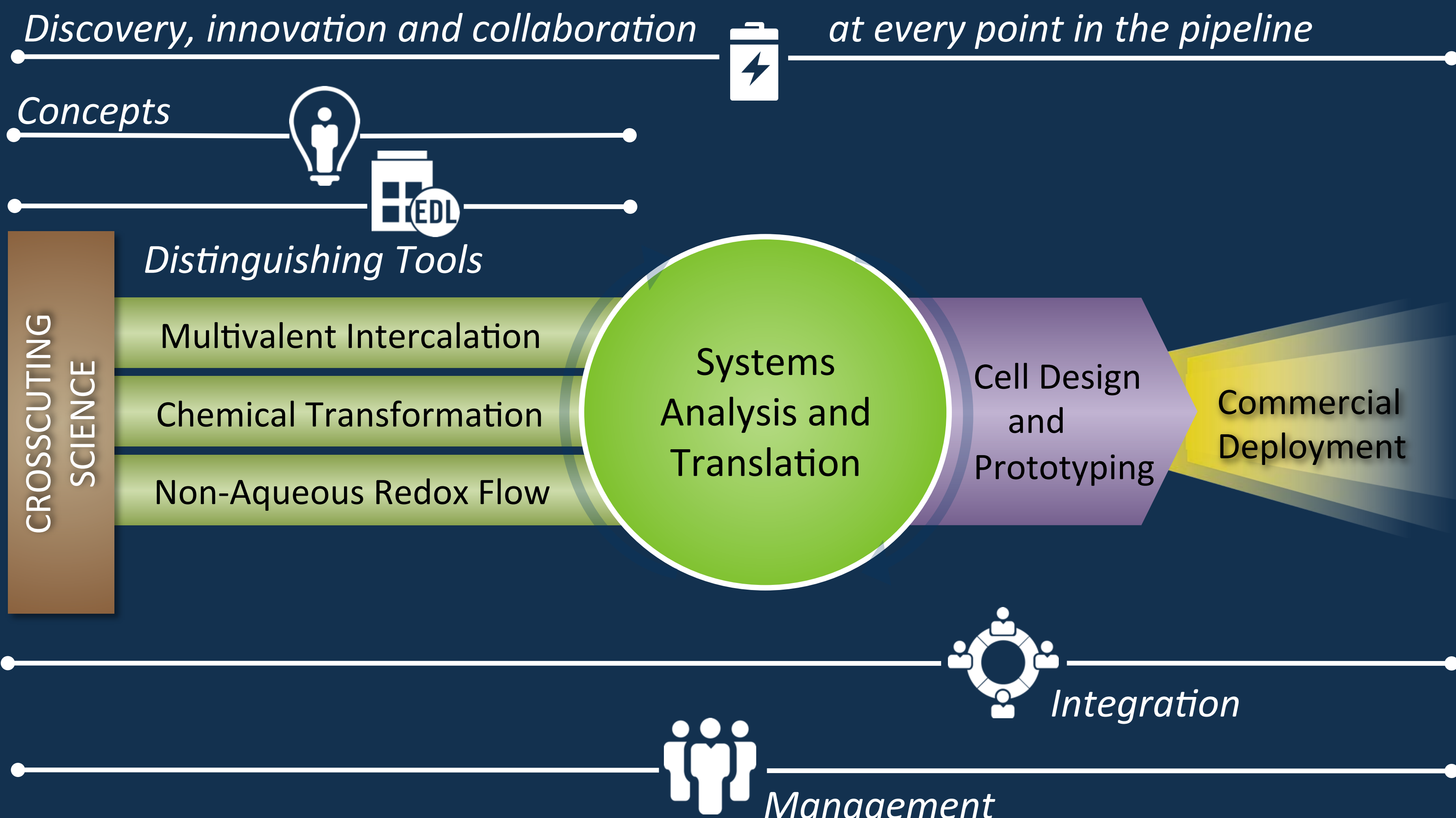


Licenses to materials cell manufacturers and automobile companies

New energy storage hub offers great opportunities for discovery, innovation, and impact

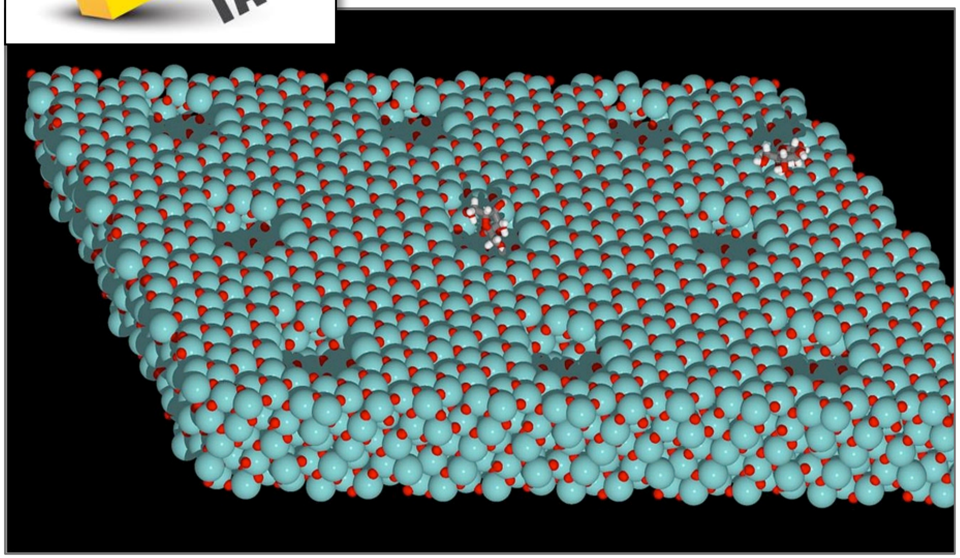
JCESR

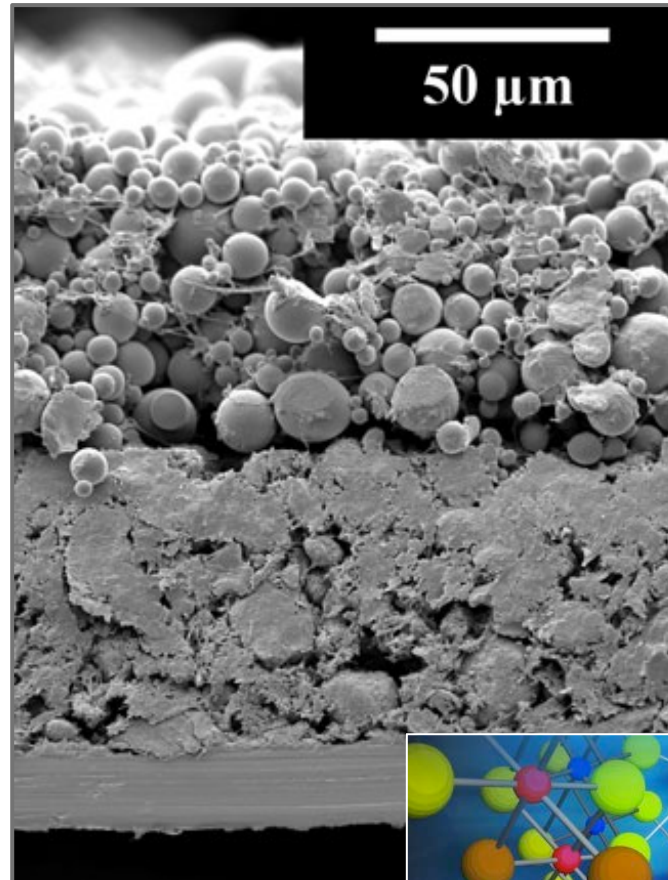
Building a new model of innovation



Argonne's EFRCs address barriers to energy production, conversion and use

`Nanobowls' allow inorganic catalysts to operate selectively on particular molecules.

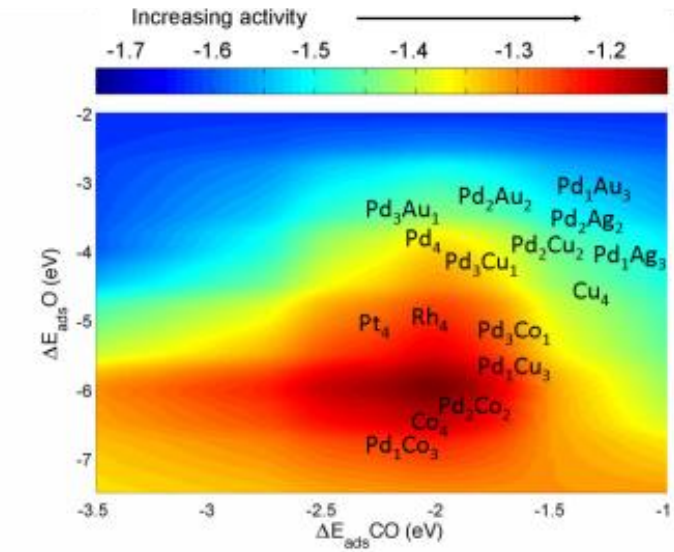




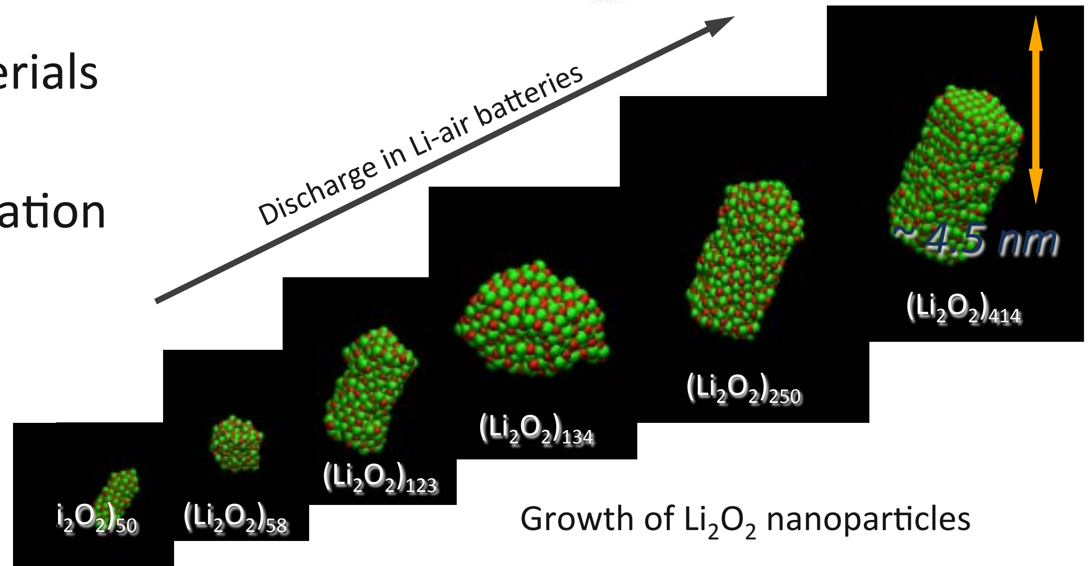
Developing `self-healing' materials to prevent thermal runaway in li-ion batteries

Computational chemistry and materials science: Designing what you make

- New and improved *ab initio* methods
- Simpler models with same/better accuracy as *ab initio*
- Effective means of multiscale computation
- Software engineering and code support
- Computation to aid materials synthesis
- Path to exascale computation

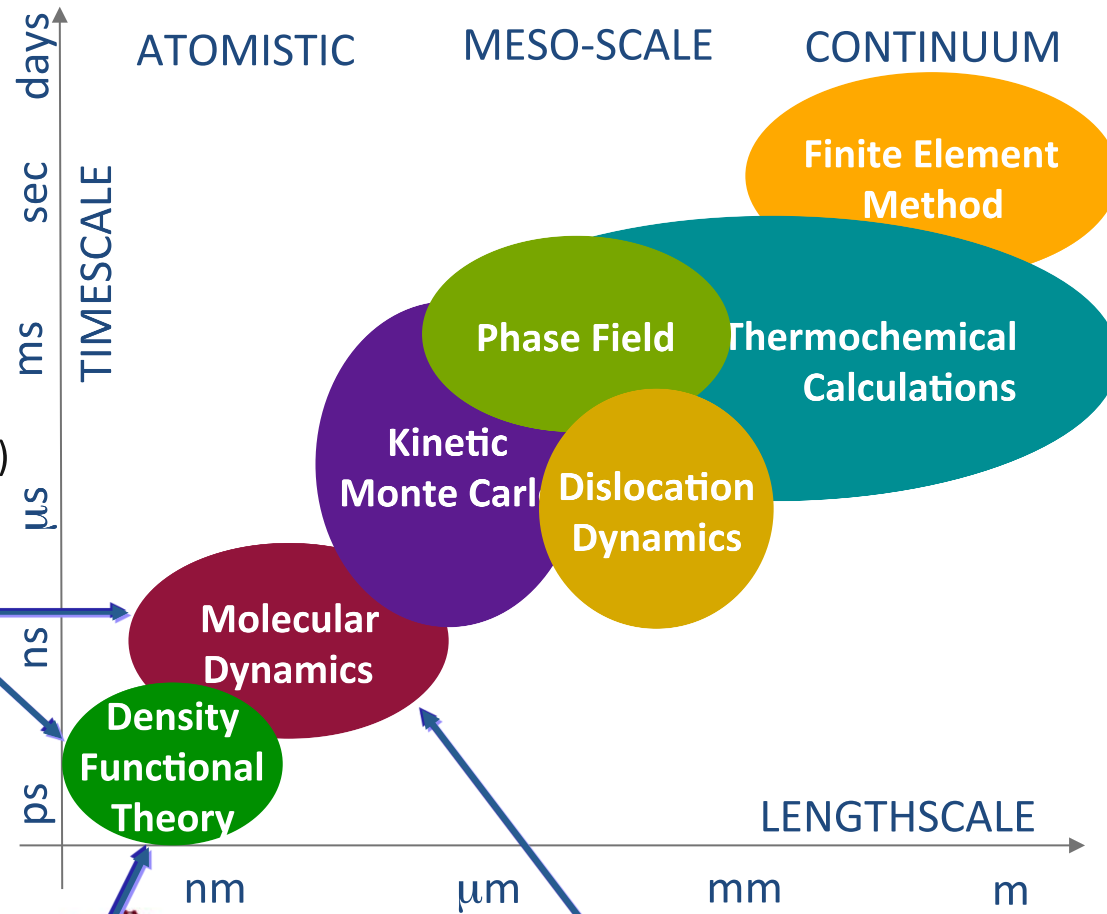


Volcano plots for screening of catalysts for Li-air batteries

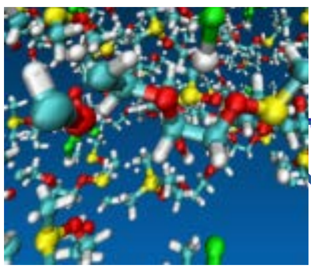


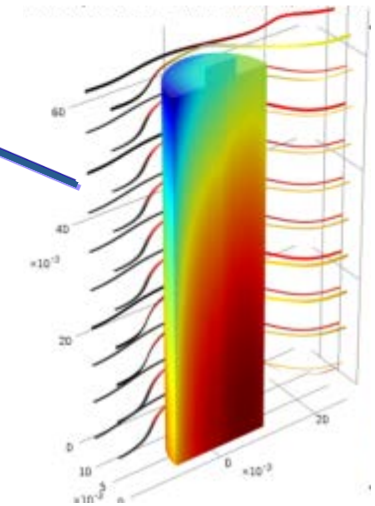
Growth of Li_2O_2 nanoparticles

Multiscale theory & computation: `Battery computer simulator'

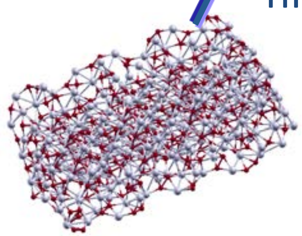


Ion diffusion in Li-air battery electrolyte (CPMD)

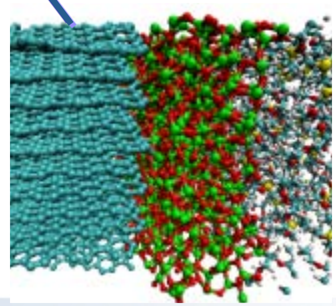




Velocity field and heat profile in an air-cooled battery (FEM)

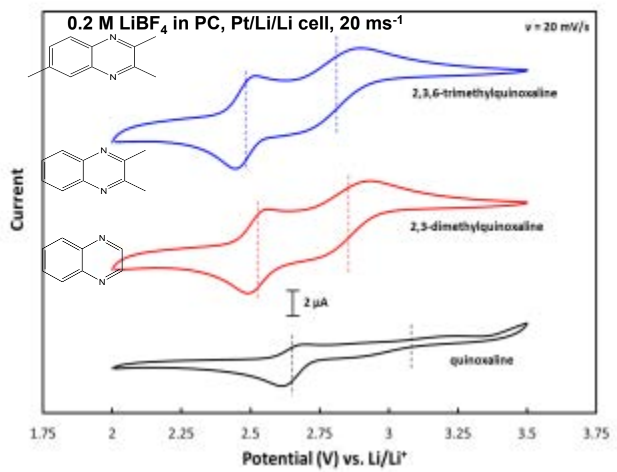


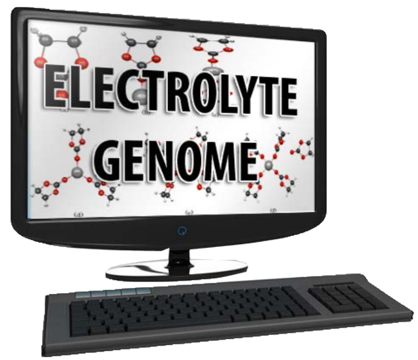
Li-peroxide nanoparticle (DFT)

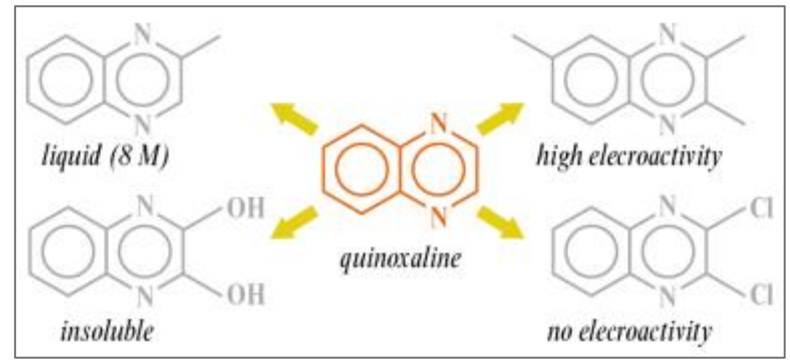


Graphite/Li_2CO_3/ electrolyte interface (MD)

Building an electrolyte genome: A new horizon for designing novel electrolytes and redox-active molecules

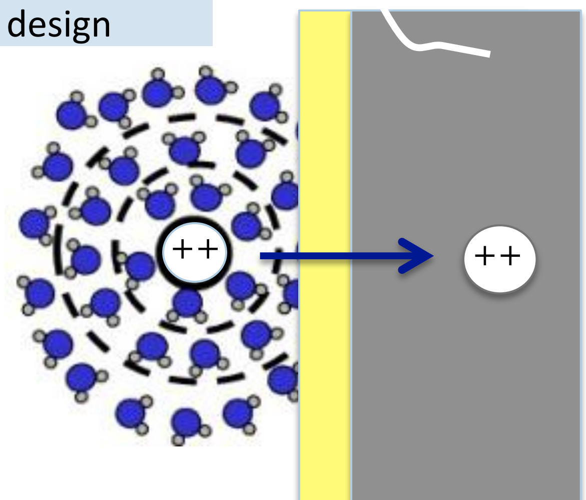




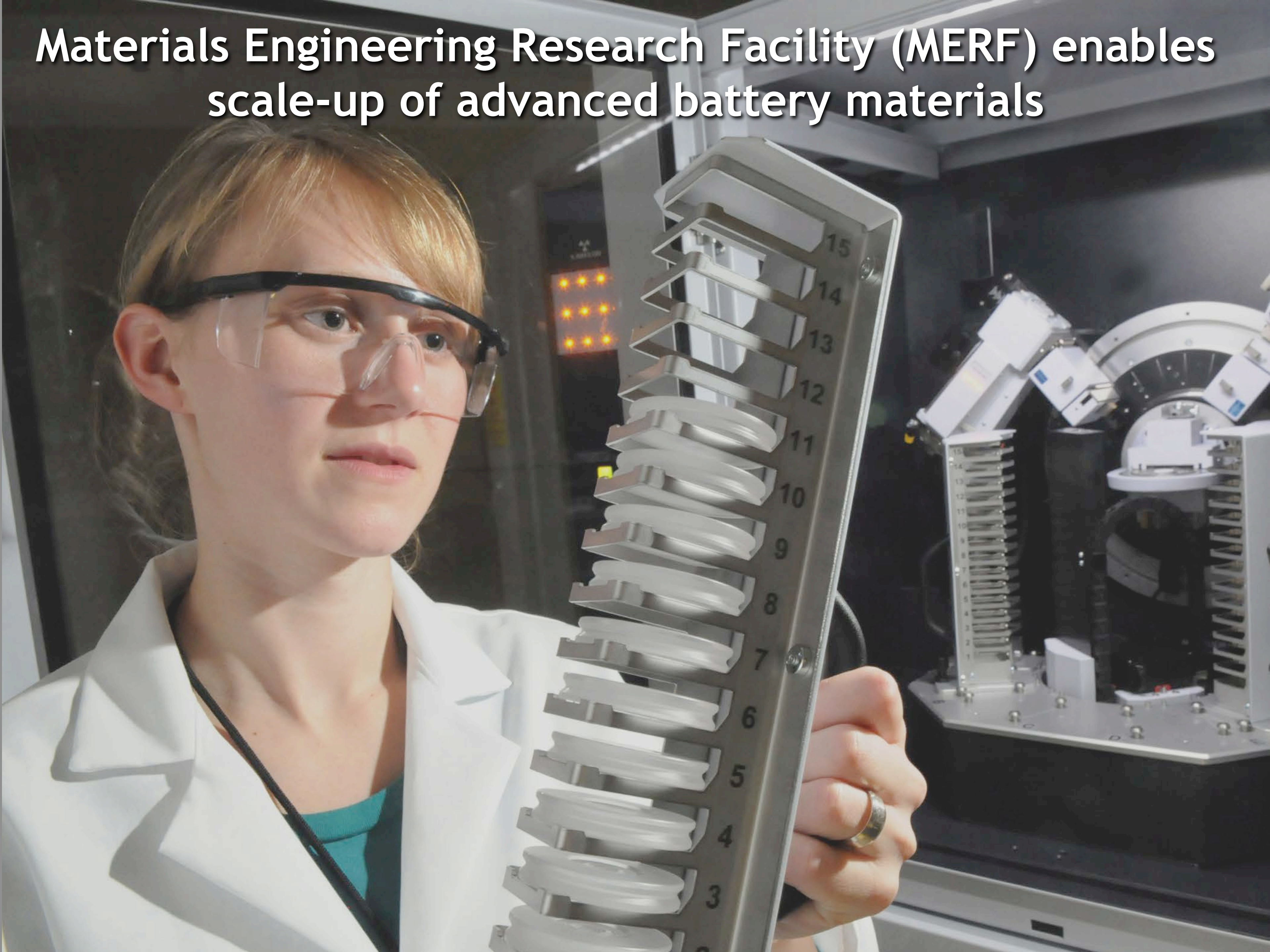


Computational structure/composition/property platform
10^4-10^5 solvents, salts, and redox molecules;
organized for interactive searching and design

- Redox activity
- Stability against cathode / anode
- Solvation structure and mobility
- Solvation / desolvation dynamics
- Solubility
- Energy storage capacity



Materials Engineering Research Facility (MERF) enables scale-up of advanced battery materials

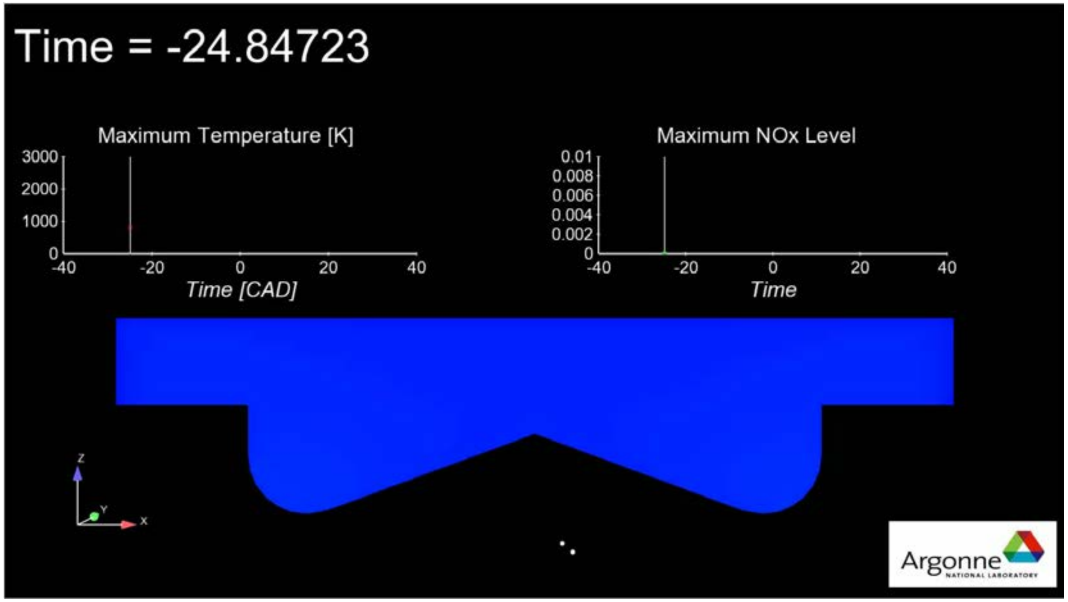


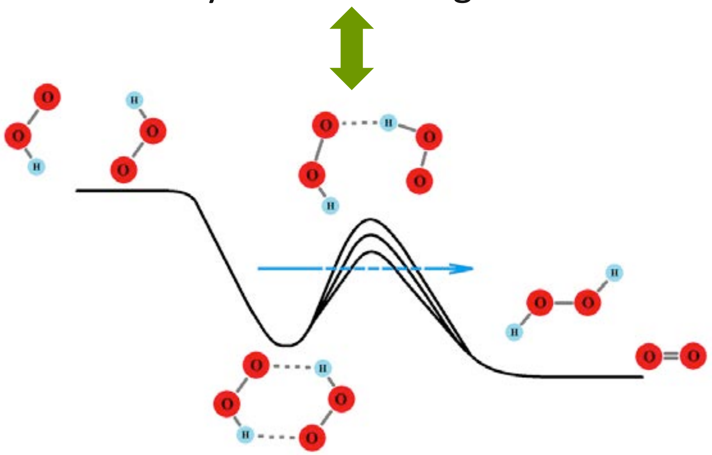
Argonne's transportation research program is world-renowned

Intelligent engine design strategy

- Creating virtuous cycle of chemistry, simulation and engineering in engines
- Combustion simulations with a biofuel/diesel blend show a strong dependence on the rate constants of several fundamental chemical reactions
- Towards the 'virtual engine'

Modeling Caterpillar single cylinder test engine

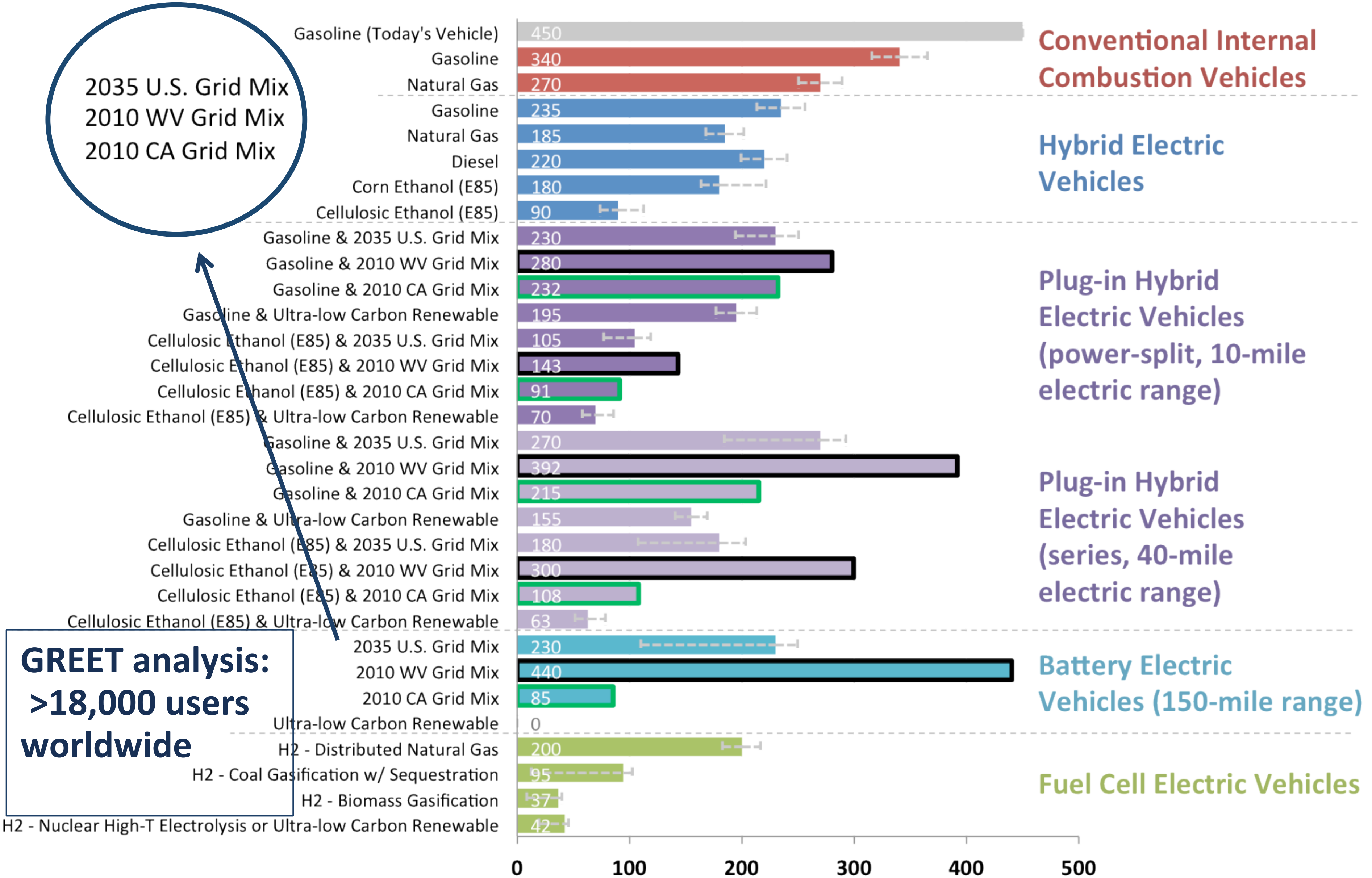




Potential energy surface for HO_2 + HO_2 + HO_2 = H_2O_2 + O_2

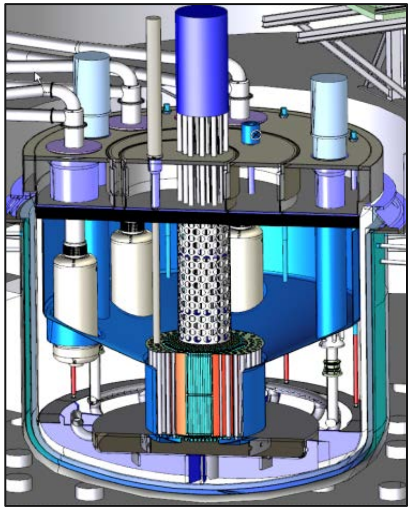
Fundamental quantum effects can influence predictions from engine simulations

Well-to-wheels analysis enables effective energy policies

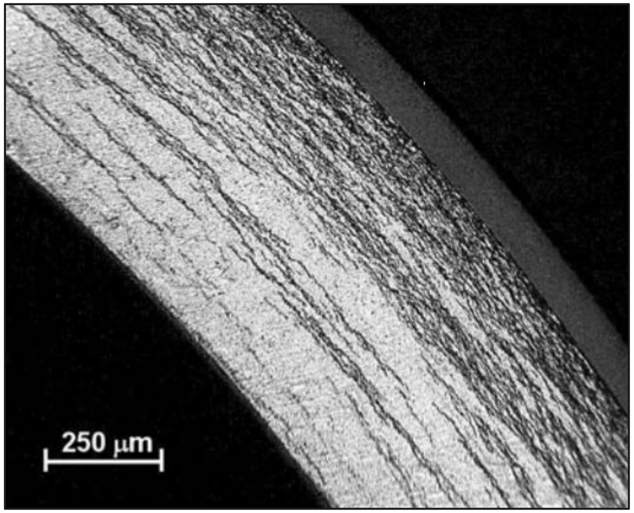


Argonne's roles in enabling future of nuclear energy

Argonne facility for studying passive cooling of reactor vessels during postulated accidents



Design concept for a small, modular burner reactor



Cross section optical micrograph of Zircaloy-4 cladding in high-burnup PWR fuel; M. Billone, ANL

Nuclear Safety

- Accident-tolerant fuels
- Corrosion of reactor materials
- Severe accident mitigation

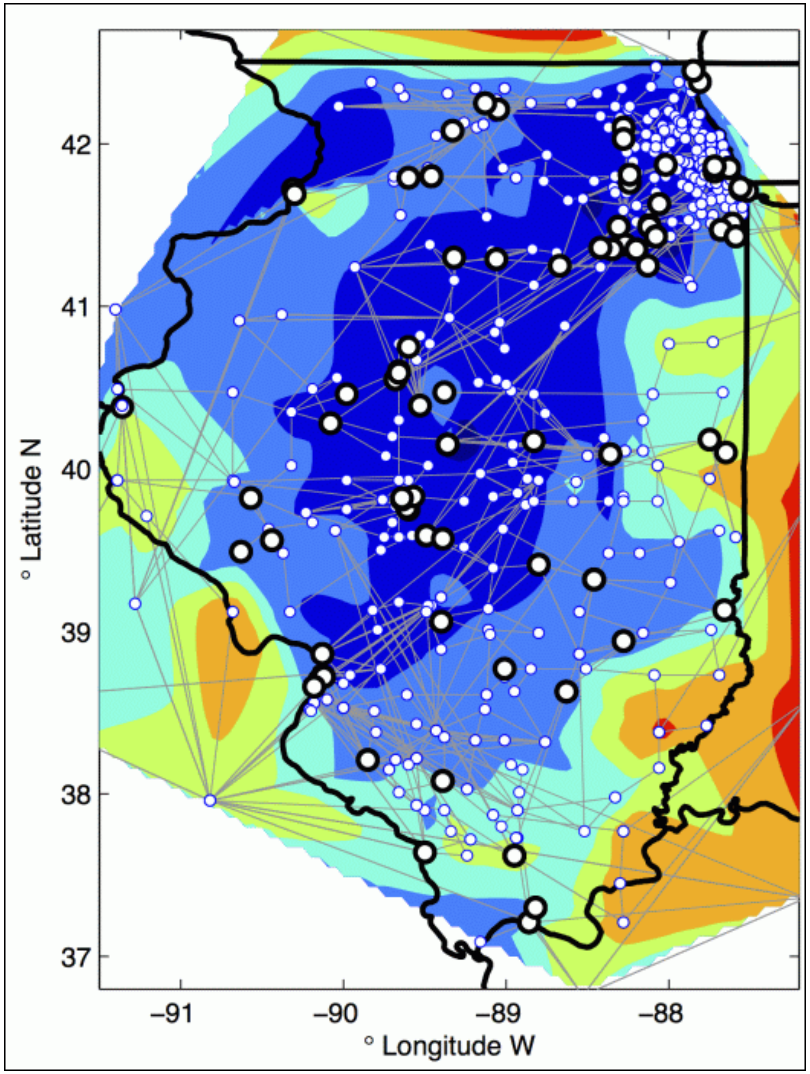
Nonproliferation

- Fast burner reactor technologies
- Safeguards for reprocessing
- LEU conversion of research and medical isotope facilities (NNSA)

Nuclear Waste

- Cladding and fuel performance
- Geologic disposal concepts
- Advanced fuel cycles

Our major research initiatives are supported, expanded by wide-ranging computational ecosystem



Mihai Anitescu et al.

Grid optimization simulation

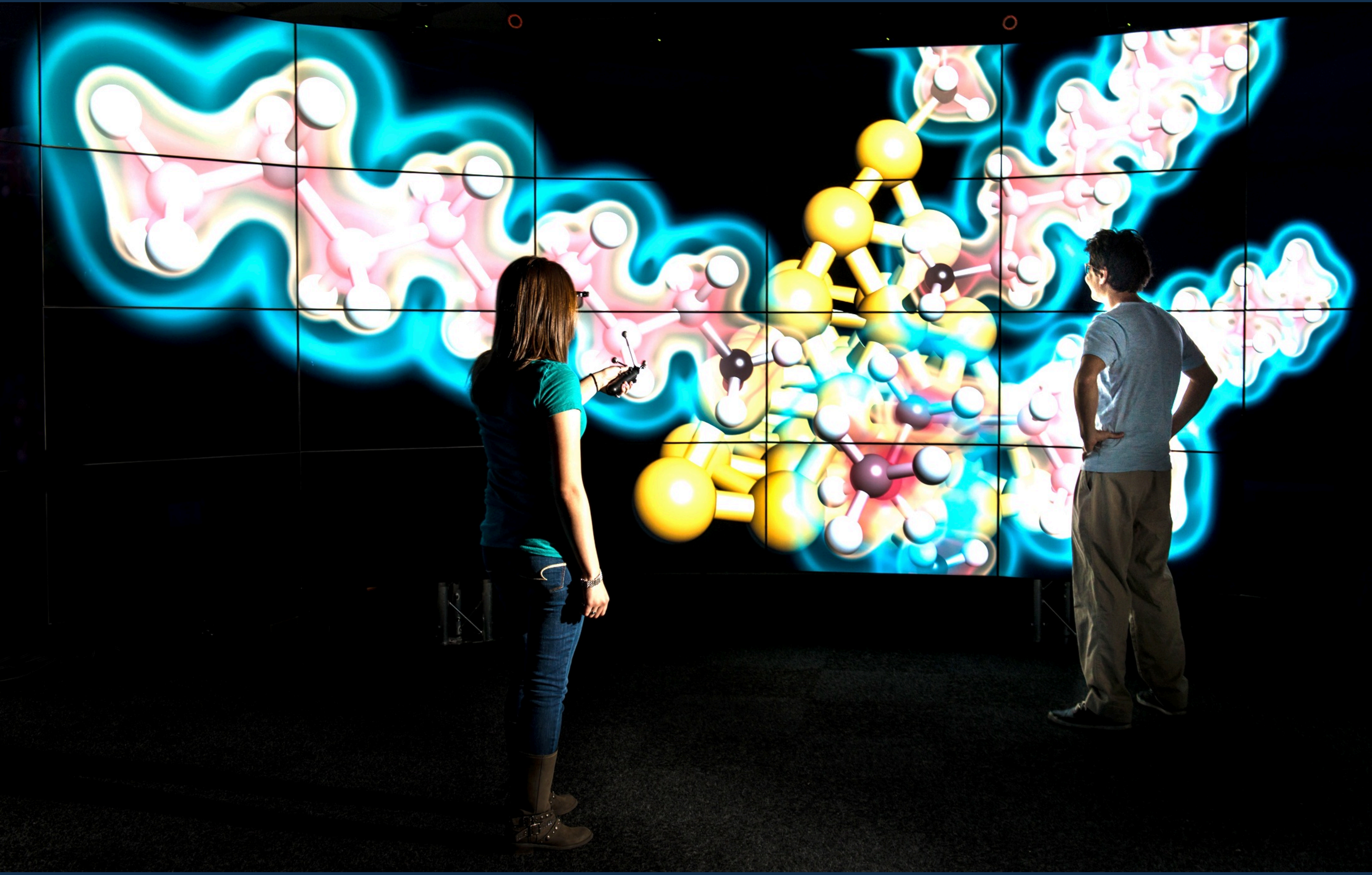
Stochastic programming formulation for Illinois:

- 2,000 transmission nodes
- 2,500 transmission lines
- 900 demand nodes
- 300 generation nodes
- Considered over 24 successive hourly time periods
- Simulation can reach billions of variables/constraints

Result

Up to 20% wind penetration can be accommodated without significant reserve increase (e.g., peaker plants) if using stochastic optimization

Argonne's scientist and engineers: Seeking the next big idea…



Thank you