Computational Materials Science and Chemistry for Innovation

Interim Report from the ASCR–BES Workshop

Presented to

Advanced Scientific Computing Advisory Committee

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Outline

- National context
- The challenge of complexity
- Simulation-based engineering and science
- Workshop approach and themes
- Materials and chemistry by design: Why now?
- Creating an innovation ecosystem

Advances in materials and chemistry have shaped history

Materials lend their names to ages

- Stone
- Bronze
- Iron
- Nuclear
- Silicon

Advances have shifted the economic and military landscape

- Iron and steel
- Gunpowder
- Ammonia synthesis
- Uranium and plutonium
- Silicon-based electronics

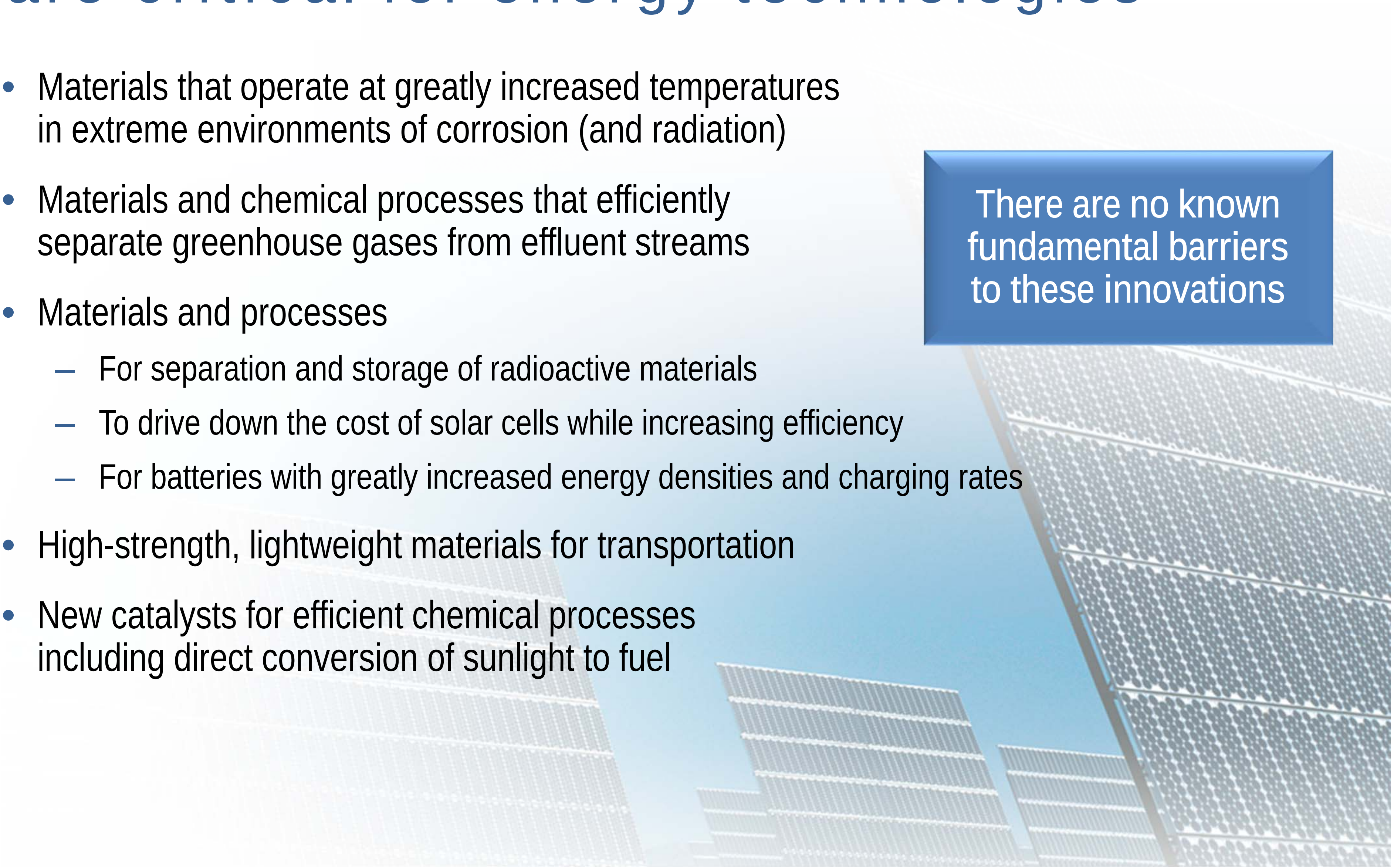
Materials and chemistry provide a pathway to innovation

Energy technologies are limited by the availability of advanced materials and chemical processes

- More than 100 years since the invention of the solar cell, electric car, and rechargeable battery
- Fossil plants operate at two-thirds optimum efficiency
- No consensus on nuclear fuel cycles or disposal of spent fuel

None of these technologies
are close to meeting their potential

Transformational advances in materials and chemistry are critical for energy technologies



- Materials that operate at greatly increased temperatures in extreme environments of corrosion (and radiation)
- Materials and chemical processes that efficiently separate greenhouse gases from effluent streams
- Materials and processes
  - For separation and storage of radioactive materials
  - To drive down the cost of solar cells while increasing efficiency
  - For batteries with greatly increased energy densities and charging rates
- High-strength, lightweight materials for transportation
- New catalysts for efficient chemical processes including direct conversion of sunlight to fuel

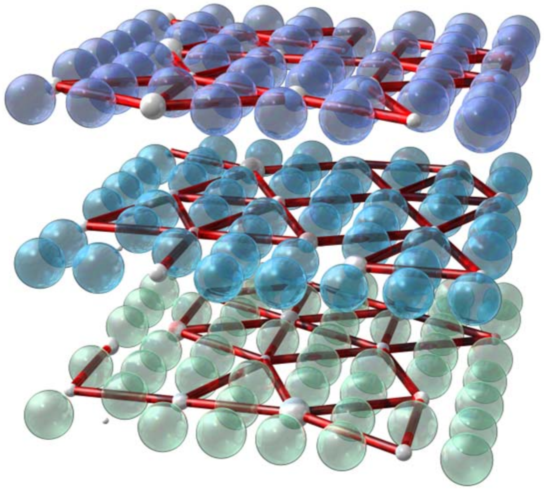
There are no known fundamental barriers to these innovations

Materials science and chemistry also underpin industrial competitiveness

- Progress in virtually all technologies depends on advances in materials and chemistry
- The company or nation with the best environment for discovering and deploying new materials and chemical processes will be more competitive
- Transformative advances in materials and chemistry will be achieved:
  The question is how quickly and by whom?

The challenge of complexity

- Achieving performance gains requires exploiting many degrees of freedom in composition and structure
- The parameter space for advanced steels has increased a million-fold compared to early steels
- There are billions of chemical combinations and structures for new catalysts
- New superconductors and high-field magnets are much more complex than their predecessors
- Intuitive, “trial and error” discovery is impractical



We do not have the time or resources to explore all the options experimentally

Transforming the discovery process

- Over the past 2 decades, the U.S. has developed and deployed the world's most powerful collection of tools for the synthesis, processing, characterization, and simulation and modeling of materials and chemical systems at the nanoscale
  - World-leading x-ray and neutron sources
  - Nanoscale science centers
  - High-performance computers
- For the first time in history, we are able to synthesize, characterize, and model materials and chemical behavior at the length scale where this behavior is controlled
- This transformational leap conveys a significant competitive advantage

Simulation–based engineering and science (SBES)

- Over the past decade, computing power has increased by a factor of 1,000
  - U.S. leads with 7 of the top 10 machines including 1, 3, and 4
- In the same period, software advances have added another factor of 1,000 for many applications
- This million-fold increase in effective capability provides access to length scales, time scales, and numbers of particles that transform our ability to understand and design new materials and chemistries with predictive power
- This has profound implications for the pace of discovery and the creation of new technologies

SBES impacts the entire innovation cycle, from scientific discovery to product development

SBES: Early impacts

	Innovation	Impact
Boeing	Predictive optimization of airfoil design	7-fold decrease in testing
Cummins	New engine brought to market solely with modeling and analysis tools	Reduced development time and cost; improved engine performance
Goodyear	Predictive modeling for new tire design	3-fold reduction in product development time
Ford	Virtual aluminum casting	Estimated 7:1 return on investment; $100M in savings
GE/P&W	SBES for accelerated insertion of materials in components	50% reduction in development time, increased capability with reduced testing

SBES has demonstrated significant improvements in product development cycles across several industry sectors

Workshop on Computational Science and Chemistry for Innovation

Bethesda, Maryland, July 26–28, 2010

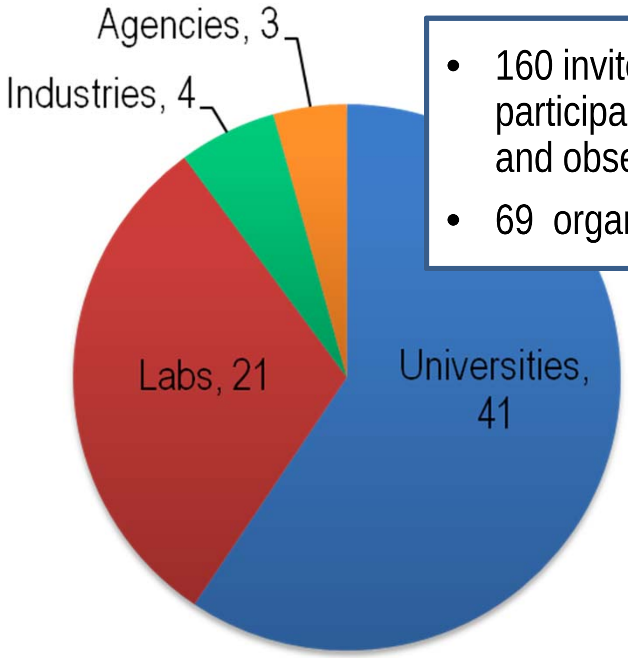
Co-chairs	• George Crabtree, Argonne National Laboratory • Sharon Glotzer, University of Michigan • Bill McCurdy, University of California–Davis • Jim Roberto, Oak Ridge National Laboratory
Sponsors	• Office of Advanced Scientific Computing Research • Office of Basic Energy Sciences

Premise

- Advances in computing and computational science offer the potential for predictive capability in many areas of science and engineering
- Experimentally validated simulations will accelerate discovery and innovation
- This provides a competitive advantage for both science and technology

Approach

- Assemble experts in materials, chemistry, and computational science
- Build on existing Basic Research Needs, Grand Scientific Challenges, Exascale, ICME, and FTAC reports
- Assess the potential of experimentally validated simulations to accelerate discovery and innovation
- Prepare a report
  - Describing challenges and opportunities
  - Focusing on potential impacts in science related to energy technologies
- Arrange for a power (and internet) blackout to remove all distractions



- 160 invited participants and observers
- 69 organizations

Plenary session

Welcome and introductory remarks	• Steve Koonin • Michael Strayer • Harriet Kung
Basic energy sciences context	• Basic Research Needs workshops: Harriet Kung
Computational sciences context	• Exascale, Grand Scientific Challenges, and FTAC workshops: Paul Messina (ANL), Thom Dunning (Illinois), Chuck Romine (NIST)
Industrial context	• Integrated computational materials engineering: John Allison (Ford)
Computational design of materials	• Materials Genome Project: Gerd Ceder (MIT)
Accelerating the innovation cycle	• Designing a national research initiative: Tom Kalil (OSTP)

Breakout sessions

Materials for extreme conditions	John Sarrao (LANL) Richard LeSar (Iowa State)
Chemical Reactions	Andy McIlroy (SNL) Alex Bell (UC Berkeley)
Thin films, surfaces, and interfaces	John Kieffer (U. Michigan) Ray Bair (ANL)
Self-assembly and soft matter	Clare McCabe (Vanderbilt) Igor Aronson (ANL)
Strongly correlated electron systems	Malcolm Stocks (ORNL) Warren Pickett (UC Davis)
Electron dynamics, excited states, and light-harvesting materials and processes	Gus Scuseria (Rice) Mark Hybertsen (BNL)
Separations and fluidic processes	Peter Cummings (Vanderbilt) Bruce Garrett (PNNL)

Key questions addressed in the breakouts

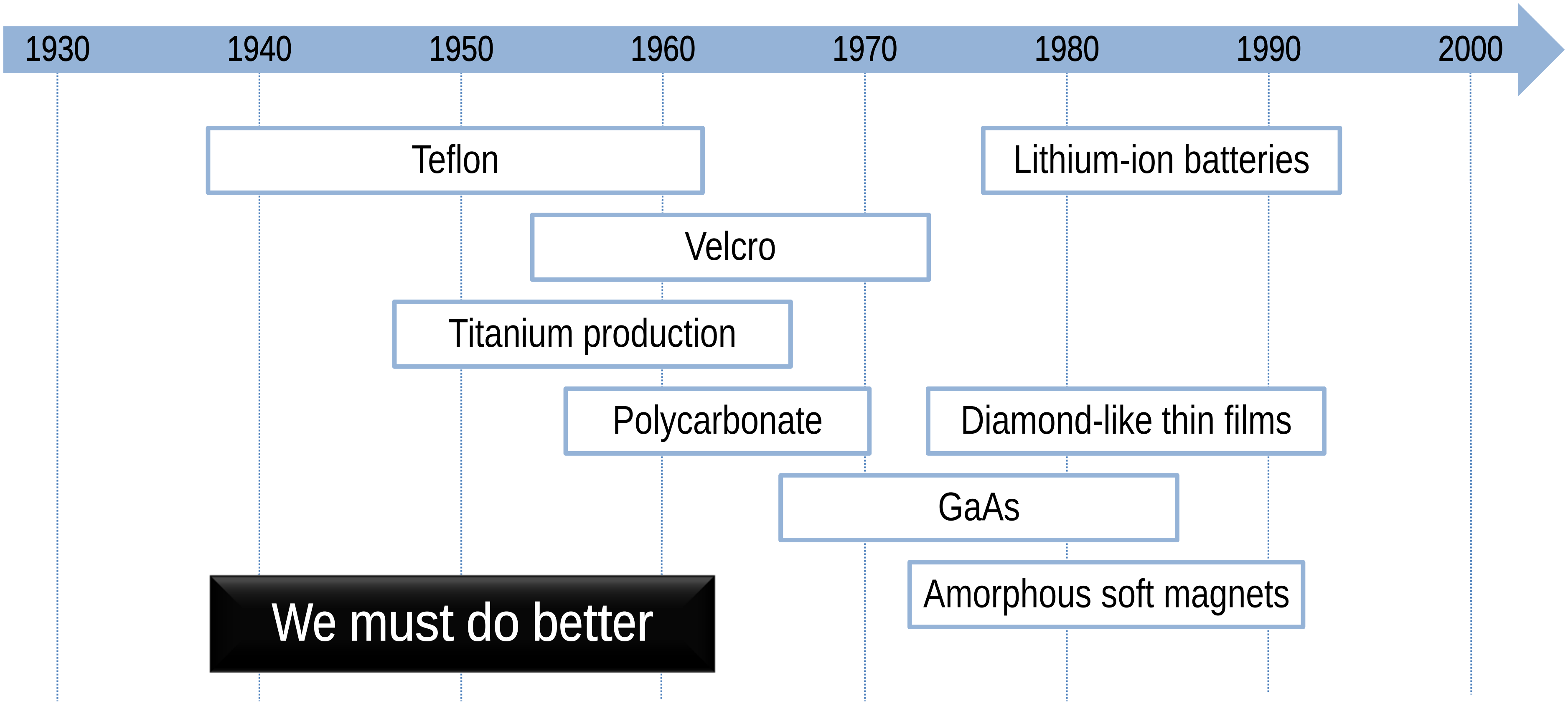
- What is the state of the art in each subfield of materials and chemistry?
- What are the most significant research opportunities/barriers in science and technology, particularly related to energy?
- How can experimentally validated computational models and simulations accelerate discovery and innovation in these areas?
- What computational and experimental challenges must be overcome to enable this acceleration?

Materials and chemistry by design: Why now?

- The experimental and computational facilities are in place
- The availability of new materials and chemistries is the pacing factor in the development of many new technologies
- Computational capability in design and manufacturing has “left the materials field in the dust”
- Predictive design of materials and chemical processes is key to accelerating the discovery and innovation cycles
- Advances are urgently needed for economic competitiveness and energy technologies

The scale and quality of U.S. scientific infrastructure currently convey a significant competitive advantage

An average of 2 decades from discovery to commercialization

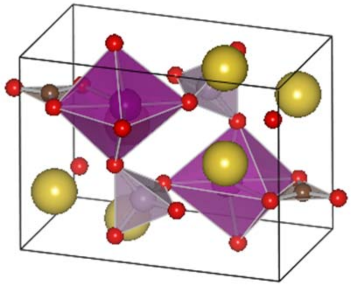


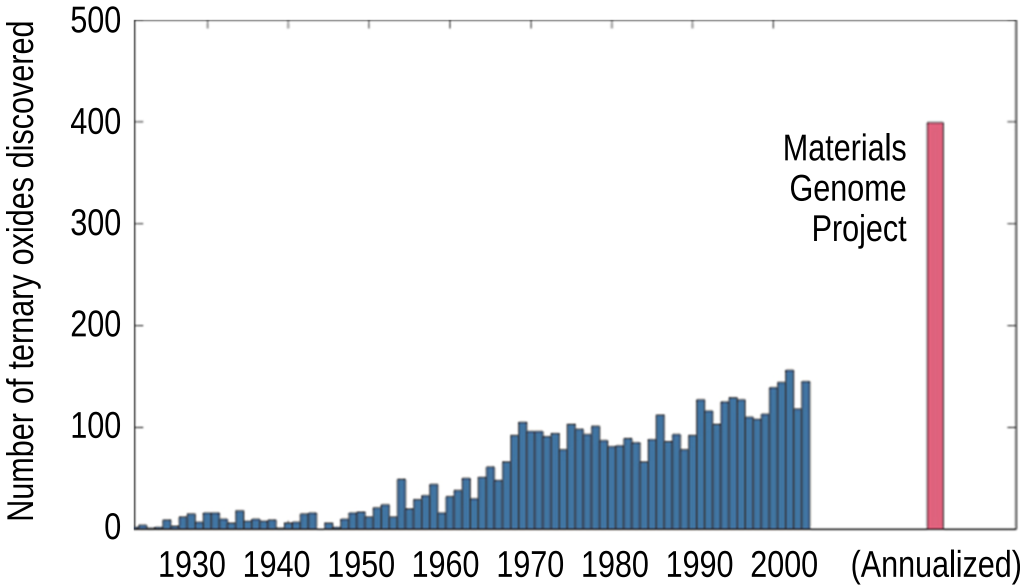
We must do better

After Gerd Ceder (MIT); materials data from T. W. Eagar and M. King, Technology Review 98 (2), 42 (1995)

Materials Genome Project: Innovative approach to accelerating the design of new materials

- Many materials properties can be predicted from first principles (more properties will become tractable with computational advances)
- Compute these properties for all inorganic compounds (approximately 100,000)
- Discover new structures and chemical classes
- Synthesize and characterize the most promising materials
- Early results: 200 new ternary compounds, new battery materials—all hundreds of times faster than conventional approaches
- “Software equals infrastructure”





Gerd Ceder (MIT)

Foundational challenges in predictive materials science and chemistry

Predicting and optimizing structure	Materials for extreme conditions
Understanding and controlling self-assembly	Designing and engineering materials at the nanoscale
Light harvesting	Photons to energy
Controlling chemical reactions	Combustion and designer catalysts
Separations and carbon capture	Chemical engineering by design
Designer thin films and interfaces	From interfacial materials to advanced batteries
Predicting and controlling electronic structure	From spins to superconductivity

Creating an innovation ecosystem

- Integration of synthesis, processing, characterization, and simulation and modeling
- Achieving/strengthening predictive capability in foundational challenge areas
- Developing computational approaches that span vast differences in time and length scales
- Validation and quantification of uncertainty in simulation and modeling
- Robust and sustainable computational infrastructure, including software and applications
- Efficient transfer and incorporation of SBES in industry

Goal: Accelerate discovery and innovation through predictive materials science and chemistry