U.S. DEPARTMENT OF ENERGY | Office of Science

BES Virtual Roundtable on "Foundational Science to Accelerate Nuclear Energy Innovation"

July 20-22, 2022

Co-Chair: Blas Uberuaga
Los Alamos National Laboratory

Co-Chair: Marianne Walck
Idaho National Laboratory

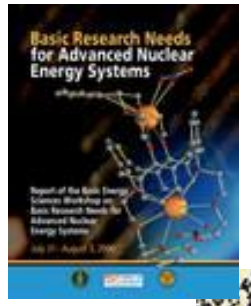
Co-Chair: Rebecca Abergel
University of California Berkeley
Lawrence Berkeley National Laboratory

Briefing to the Basic Energy Sciences Advisory Committee - December 7, 2022

Previous DOE Reports and Initiatives

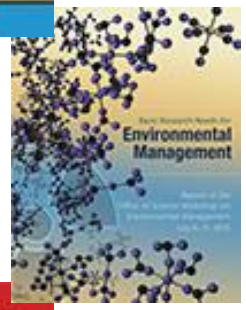
BES Basic Research Needs for **Advanced Nuclear Systems**

August 2006; Co-Chairs: Jim Roberto (ORNL) and Tomas Diaz de la Rubia (LLNL)



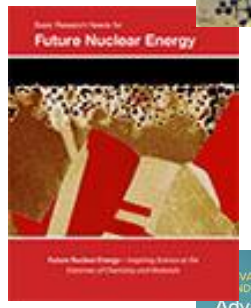
BES Basic Research Needs for **Environmental Management**

July 2015, Co-Chairs: Sue Clark (PNNL/WSU), Michelle Buchanan (ORNL), Bill Wilmarth (SRNL)



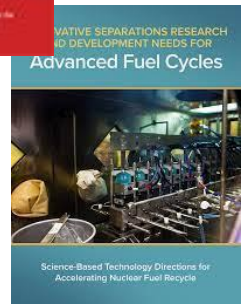
BES Basic Research Needs for **Future Nuclear Energy**

August 2017, Co-Chairs: Kelly Beierschmitt (INL), Michelle Buchanan (ORNL), Aurora Clark (WSU), and Ian Robertson (UW Madison)



NE Innovative Separations R&D Needs for **Advanced Fuel Cycles**

August 2021, Co-Chairs: Bruce Moyer (ORNL) and Gregg Lumetta (PNNL)



Roundtable on Foundational Science to Accelerate Nuclear Energy Innovation – July 20-22, 2022 (Virtual)

Organized by SC-BES in coordination with NE, SC-FES and SC-ASCR

Goal: Identify the key underpinning science needs and priority research opportunities that will accelerate research, development, and deployment of nuclear energy systems, including both fission and fusion

Scope: Assess the status of the field and identify the fundamental science bottlenecks and gaps in the fundamental understanding that limit innovation in current nuclear technologies

Participants: A diverse group of up to 35 participants, representing labs, universities, and other stakeholders

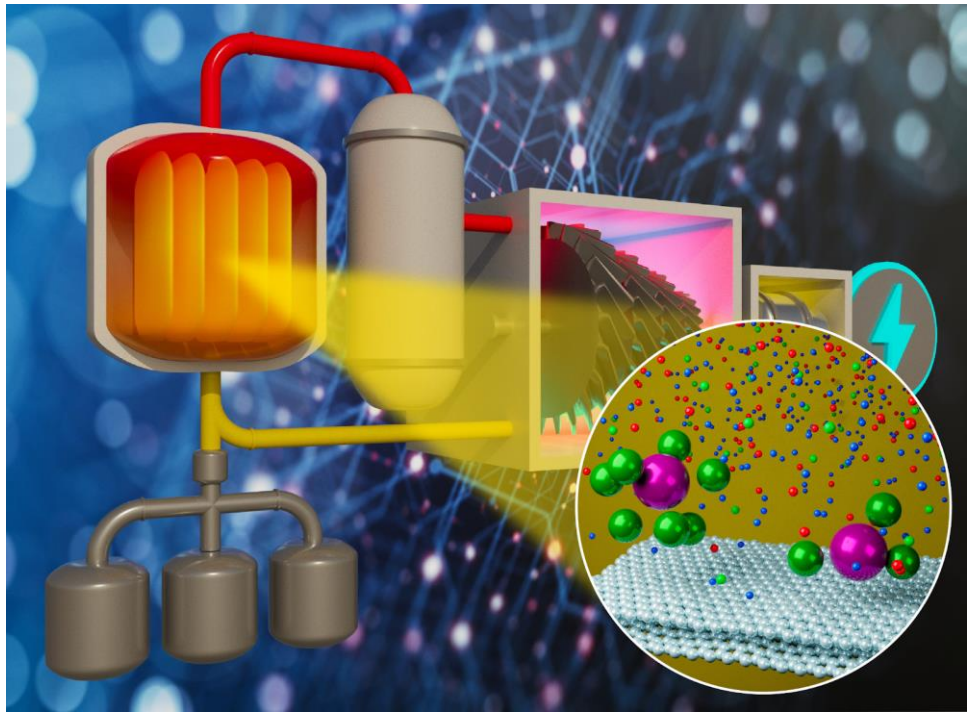


Illustration courtesy of Dr. V. Glezakou (ORNL)

Roundtable Background and Plenary Speakers

Technology Status Document Webinar

Simon Pimblott, INL

Grace Burke, ORNL

Welcome Comments

Asmeret Asefaw Berhe, DOE SC

Kathryn Huff, DOE NE

Opportunities for Advanced Computing in Accelerating Nuclear Energy Innovation: Reflections from CASL and Exascale

Doug Kothe, ORNL

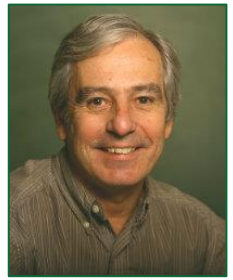
Commercial Perspective on Future Research Needs

Christine King, INL

Roundtable Panels

- **Materials Discovery and Resilience**
  Panel Lead: Janelle Wharry, Purdue

- **Physical Processes and Chemical Evolution**
  Panel Lead: Jay LaVerne, Notre Dame

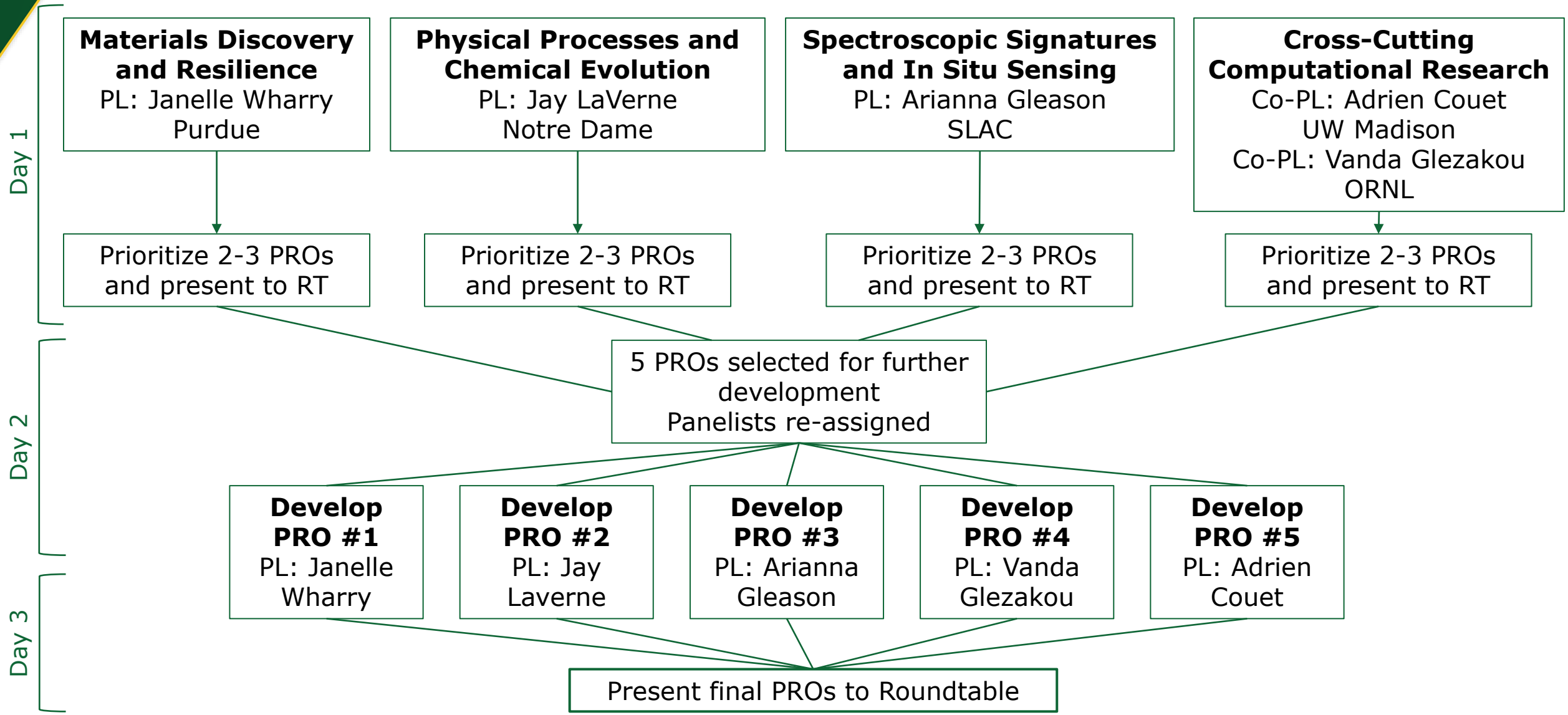


- **Spectroscopic Signatures and In Situ Sensing**
  Panel Lead: Arianna Gleason, SLAC

- **Cross-Cutting Computational Research**
  Panel Co-Leads: Adrien Couet, UW Madison
  Vanda Glezakou, ORNL

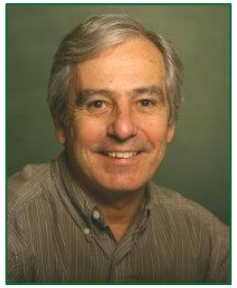
*Roundtable participants represented Universities (16) and National Laboratories (13)

Path to define Priority Research Opportunities (PROs)



Panelists Re-Aligned to Finalize Five PROs

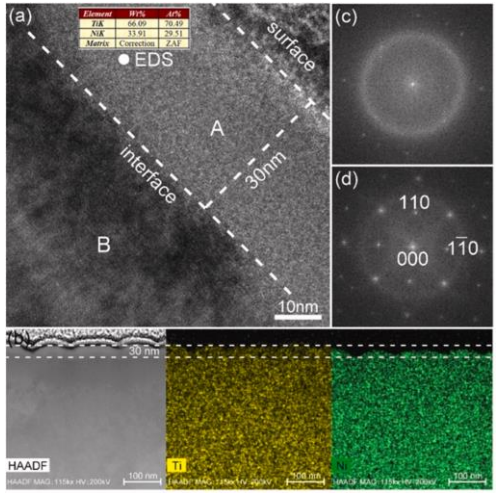
PRO #1	PRO #2	PRO #3	PRO #4	PRO #5
Complex electronic structure in novel materials	Next generation coolants and solvents	Complex interfaces in nuclear environments	Novel techniques to probe dynamic behavior	AI for self-resilient condensed phases
Lead: Wharry	Lead: LaVerne	Lead: Glezakou	Lead: Gleason	Lead: Couet



Priority Research Opportunities to Advance Foundational Science for Nuclear Energy Innovations

PRO 1: Master complex electronic structures to tailor thermochemical reactivity, transport, and microstructural evolution

Key question: How do we elucidate, predict, and harness coupled electron-ion dynamics to enable discovery and deployment of novel materials, coolants, and solvents for future fission and fusion energy?



[DOI: 10.1016/j.intermet.2021.107305]

PRO 2: Interrogate and direct the physics and chemistry underpinning next generation coolants and solvents

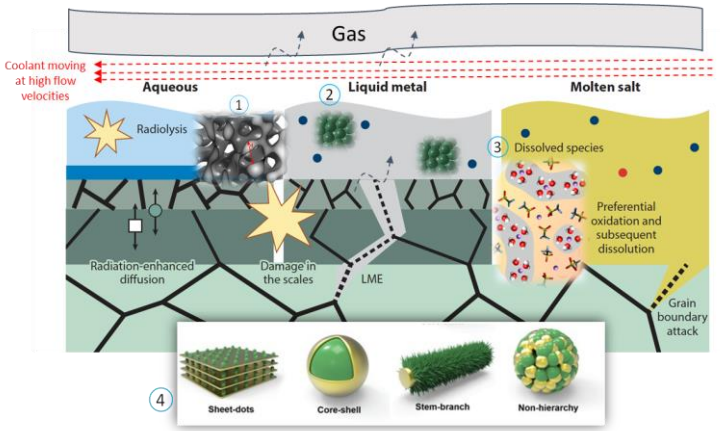
Key question: How can we probe and control the physics and chemistry of coolants, solvents and their solutions in the harsh environments associated with nuclear energy?

[DOI: 10.1002/chem.201904677]

Priority Research Opportunities to Advance Foundational Science for Nuclear Energy Innovations

PRO 3: Elucidate and control the underlying physics and chemistry of interfaces in complex nuclear environments

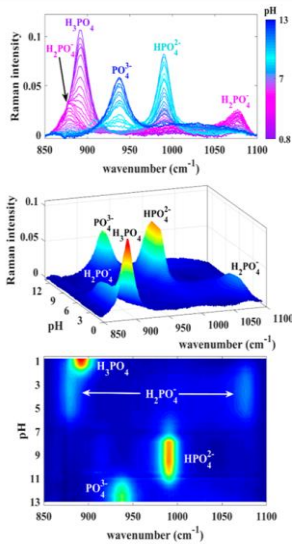
Key question: How do we harness dynamic interfaces to tailor robust materials and processes for next generation nuclear reactors?



[DOI: 10.1002/adma.202100855]

PRO 4: Bridge multi-fidelity, multi-resolution experiments, computational modeling, and data science to control dynamic behavior

Key question: Which novel techniques can be coupled to provide operando and in situ measurements to better understand and control dynamical properties, behaviors, and processes for extreme nuclear energy environments?

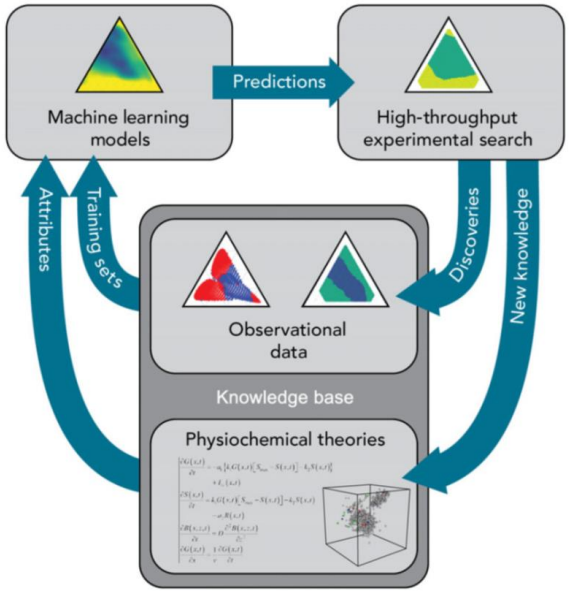


[DOI: 10.1021/acs.analchem.9b05708]

Priority Research Opportunities to Advance Foundational Science for Nuclear Energy Innovations

PRO 5: Harness artificial intelligence to design inherently resilient condensed phases

Key question: What defines self-resilient mechanisms and how can they be discovered in nuclear materials and chemical systems in coupled extreme environments?



[DOI: 10.1126/sciadv.aaq1566]

Status of Outcomes

- **Target Brochure Release:** December 2022
- **Target Report Release:** February 2023
- **Technology Status Document:** February 2023
- **Output:** A public report describing Priority Research Opportunities that identify fundamental science needs to overcome technological barriers to advanced nuclear energy systems, including both fission and fusion.

Acknowledgements

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  - Stephen Kung
  - Jon Carmack
  - Dirk Cairns-Gallimore
  - Daniel Nichols
- ORAU Staff
- ORNL Production Team
- All observers
- All panelists and panel leads

  A. Couet, A. Lines, A. Jokisaari, A. Gleason, C. Pearce, D. Perez, D. Jiang, D. Chidambaram, E. Sooby, F. Selim, G. Horne, J. Marian, J. Wishart, J. Wharry, J. Hattrick-Simpers, J. LaVerne, J. McFarlane, K. Knope, K. Peterson, M. Li, M. Furlanetto, M. Weaver, O. Anderoglu, R. Castro, R. Wilson, S. Mathaudhu, V. Glezakou

Questions?

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