U.S. DEPARTMENT OF ENERGY | Office of Science

Chemical Sciences, Geosciences, and Biosciences Division: Strategic Planning Process & Progress

Briefing to BESAC

March 23, 2018

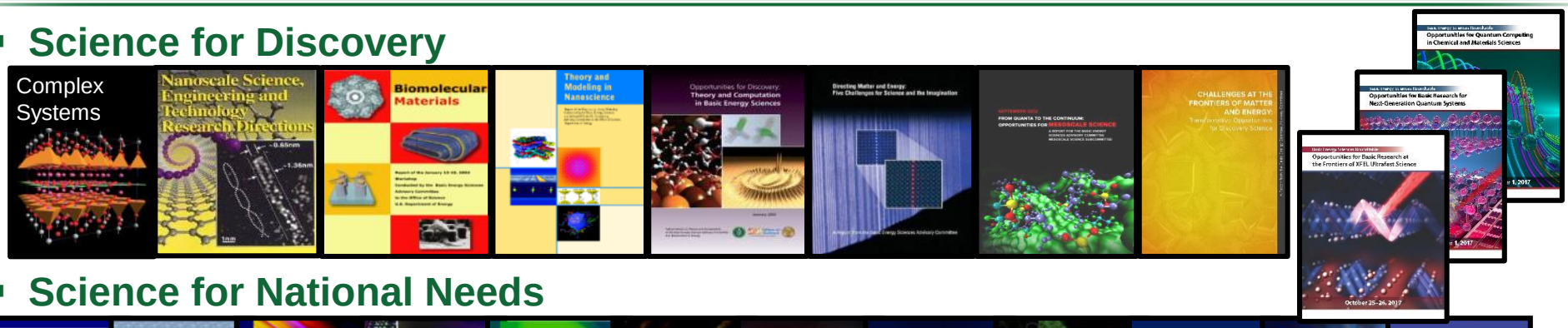
Bruce Garrett
CSGB Division Director

Strategic planning activities address major recommendations from Committee of Visitors for CSGB Division

- 2014 COV recommends "that BES *execute a strategic planning session* at the division level to evaluate current directions and *identify new opportunities and synergies*. This type of strategic planning will *facilitate communication and collaboration among the programs* …"
- 2017 The COV "commends CSGB's initial implementation of strategic planning and encourages broadening the scope to identify *synergies and new research opportunities among various CSGB teams and with other BES divisions*.

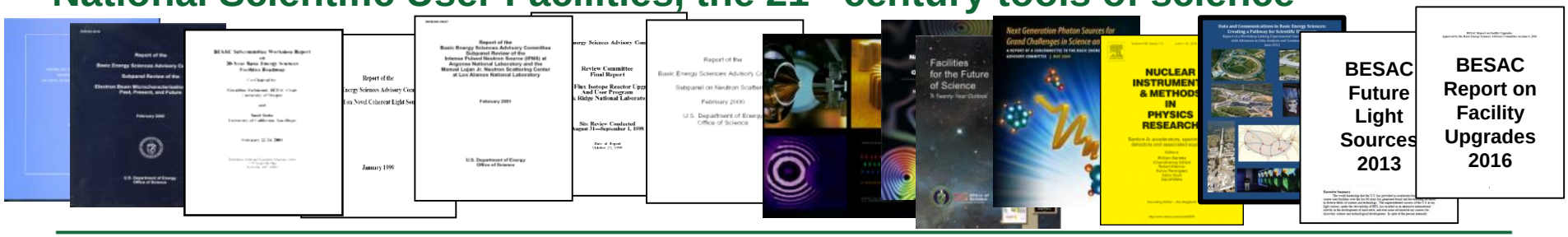
BES strategic planning activities provide the foundation for the CSGB strategy

- **Science for Discovery**



- **Science for National Needs**

- **National Scientific User Facilities, the 21st century tools of science**



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https://science.energy.gov/bes/community-resources/reports/

BES/CSGB strategic planning driven by mission/vision/goals

- **Mission**: BES/CSGB research focus is on gaining *understanding leading to control of chemical transformations and energy flow*, which provides foundations for new technologies to generate, store, and use energy and to mitigate its environmental impact
- **Vision**: Recognition of BES/CSGB for impact of scientific programs that are at the forefront of chemical sciences, geosciences and biosciences and advance DOE missions
- **Goals**:
  - Balance and synergy of discovery and use-inspired fundamental research
    - Advance ability to understand, predict, and ultimately control matter and energy
    - Surmount scientific barriers to advancing technologies
  - Innovative management of science portfolios
    - Provide focus on key and evolving scientific challenges
    - Maintain balance and health of university and lab programs; demonstrate the value and distinction of both

Strategic planning is essential to maintain health of the division's research portfolio

Community input is critical to division strategic planning

BESAC reports

BRN workshops

Roundtables

National Academy studies
(Separations Science)

Chemical Science Roundtable workshops
(Data Science: Opportunities for Chemistry)

CSGB Council workshops
(Coherence in Chem/Bio, *Nature* 543, 647, 2017)

Program Discussions
(PI meetings)

Scientific Meetings
(ACS Fed Funders)

Interagency Interactions
(e.g., EERE, FE, etc.)

Strategic planning process engages multiple levels

Division:

Plan/Execute

Teams:

Analyze/Integrate

Programs

Assess: programs, opportunities, and capabilities

Chemical Sciences, Geosciences and Biosciences Division

Bruce Garrett, Division Director

Fundamental Interactions Team

Team Lead – Jeff Krause

- **Atomic, Molecular, and Optical Sciences** — Tom Settersten
- **Gas Phase Chemical Physics** — Wade Sisk
- **Condensed Phase and Interfacial Molecular Science** — Gregory Fiechtner
- **Computational and Theoretical Chemistry** — Mark Pederson

Photochemistry and Biochemistry Team

Team Lead – Gail McLean

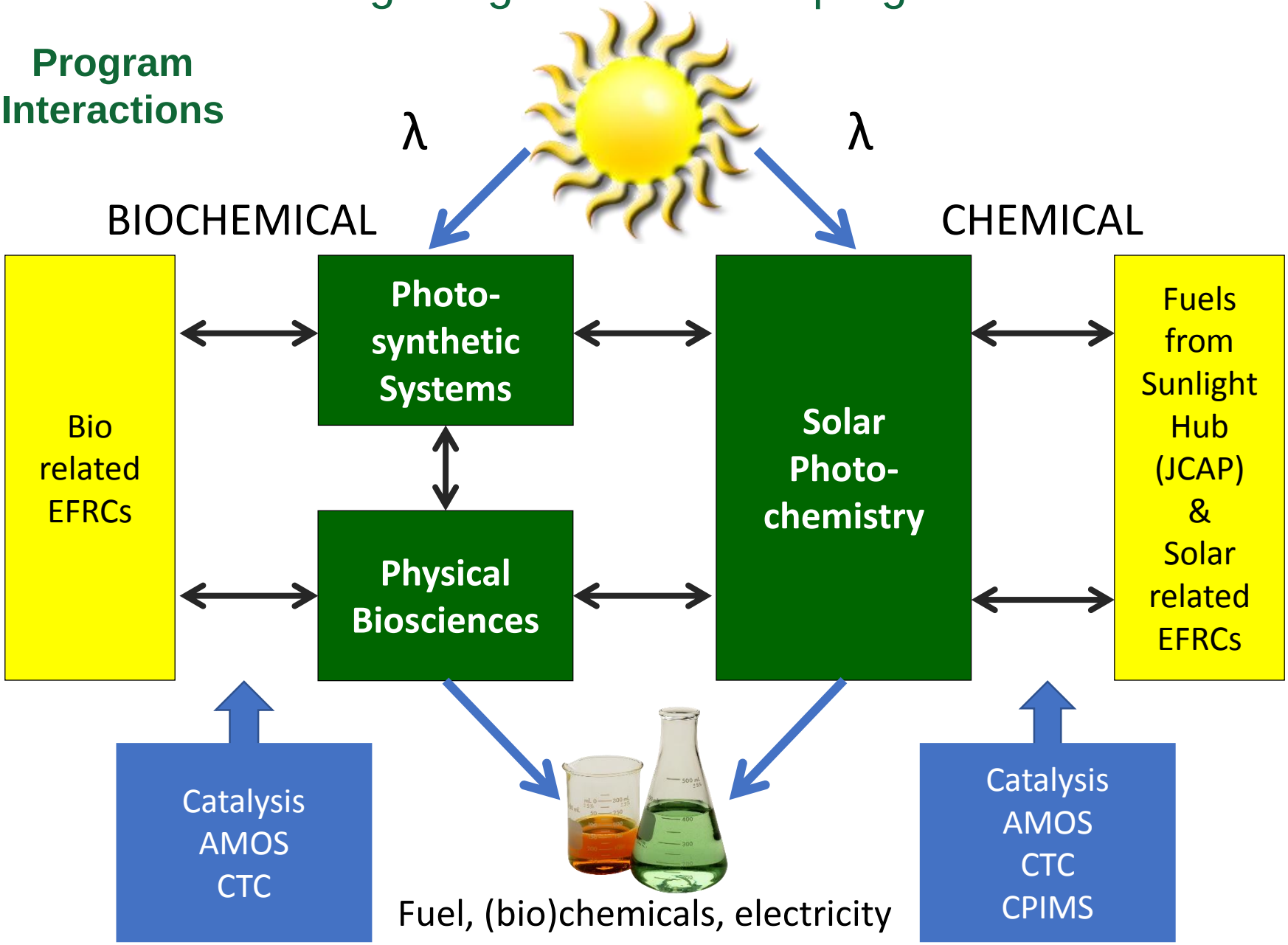
- **Photosynthetic Systems** — Stephen Herbert
- **Physical Biosciences** — Robert Stack
- **Solar Photo-chemistry** — PM vacancy
- **Fuels from Sunlight Energy Innovation Hub** — Chris Fecko

Chemical Transformations Team

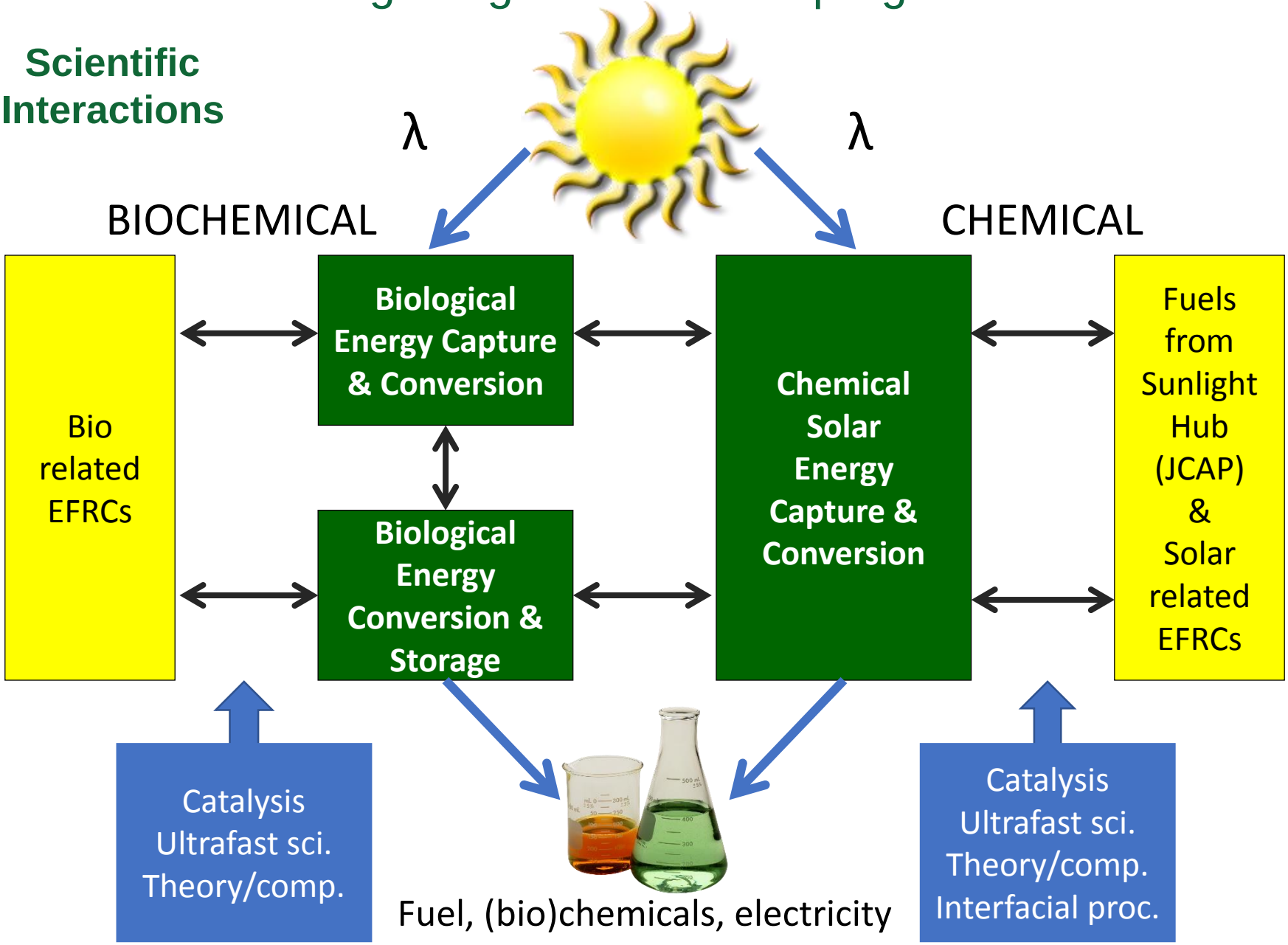
Team Lead – Raul Miranda

- **Catalysis Science** — Viviane Schwartz, Chris Bradley
- **Separation Science** — PM vacancy; Chuck Peden
- **Heavy Element Chemistry** — Philip Wilk
- **Geosciences** — James Rustad

Photochemistry and Biochemistry Team: Integrating vision across programs

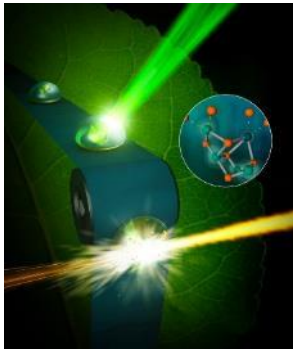


Photochemistry and Biochemistry Team: Integrating vision across programs

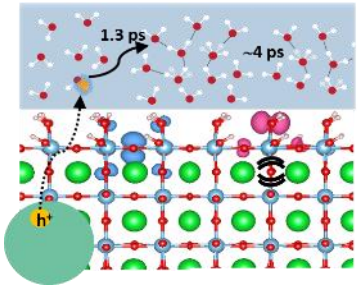


Our strategic focus is on 5 synergistic research areas at the intersection of CSGB programs

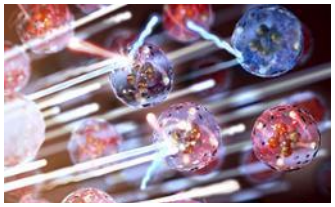
Manipulating x-rays with visible light



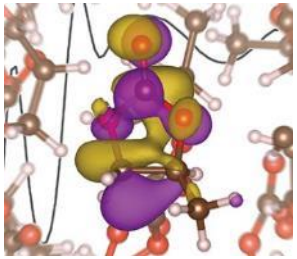
Elucidating water-splitting by Photosystem II



Elucidating charge transfer and reaction at oxide-water interface



Understanding intense x-ray–electron interactions



Modeling interactions of ions in solution

Ultrafast chemistry:
Probe dynamics of electrons, understand energy flow, elucidate structural dynamics

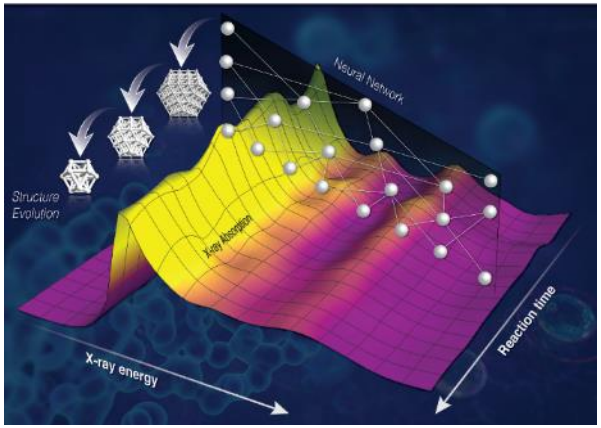
Chemistry at complex interfaces:
Uncover emergent chemical phenomena at dynamic interfaces with structural and functional heterogeneity

Charge transport and reactivity:
Elucidate contributions of charge dynamics to energy flow and its coupling to reactions

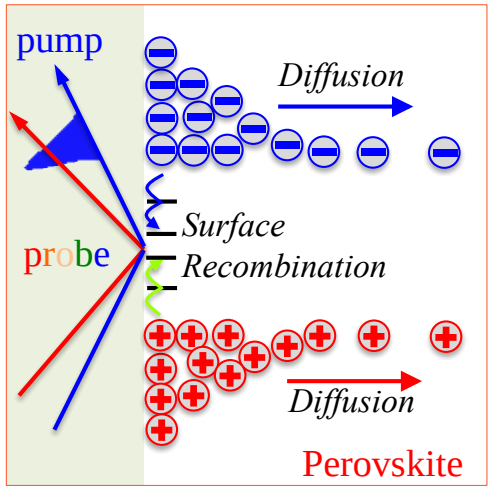
Reaction pathways in diverse environments:
Discover the influence of nonequilibrium, heterogeneous, nanoscale environments on complex reaction mechanisms

Chemistry in aqueous environments:
Address unique properties of water in extreme environments and its role in chemical phenomena

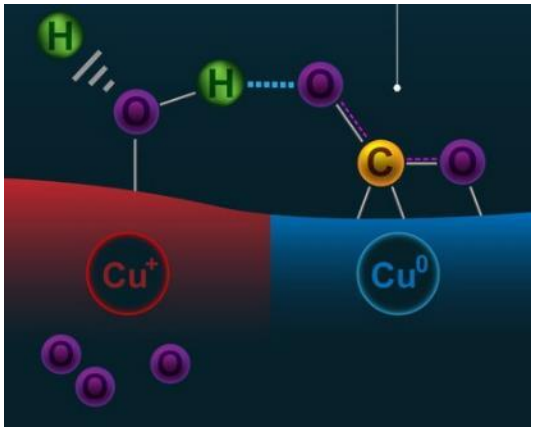
Chemistry at Complex Interfaces



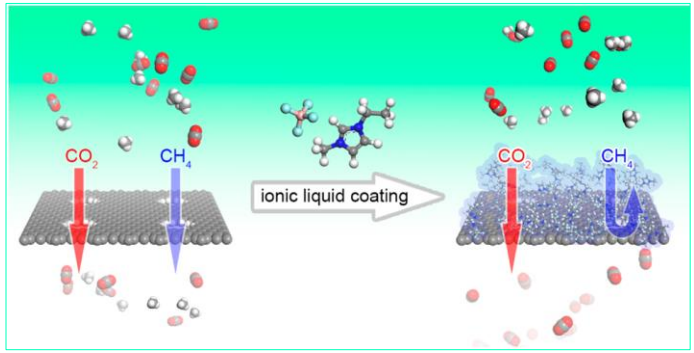
Catalysis: *Solving the structure of nanoparticles during reaction*



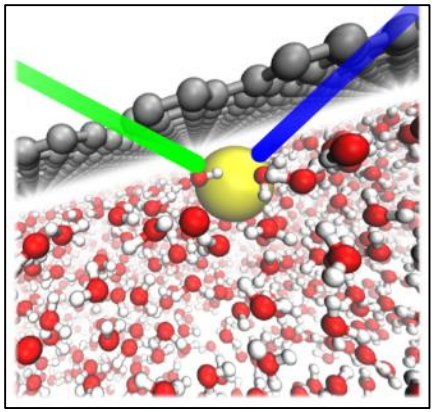
Solar Photo: *Understanding surface recombination dynamics*



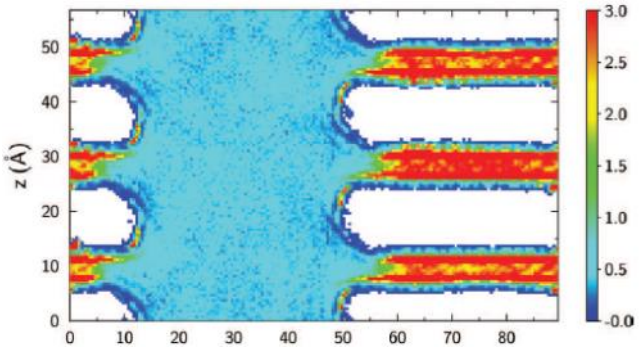
JCAP: *Revealing subsurface oxide is critical for CO_2 activation on Cu*



Separations: *Simulating ion gating to dynamically control gas separation*



CPIMS: *Unraveling mechanism of ion adsorption to aqueous interfaces*

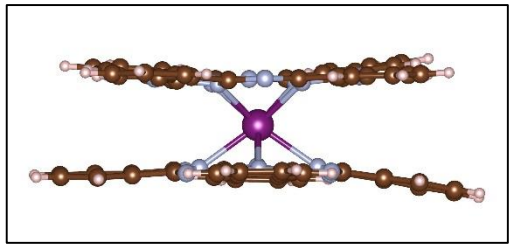


Geosci: *Understanding ion exclusion in small pores of clay minerals*

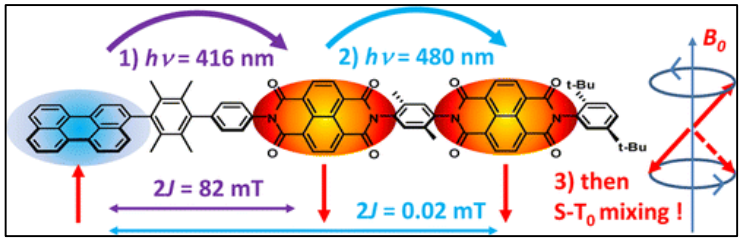
Quantum Information Science

Understand, control & exploit novel quantum behaviors

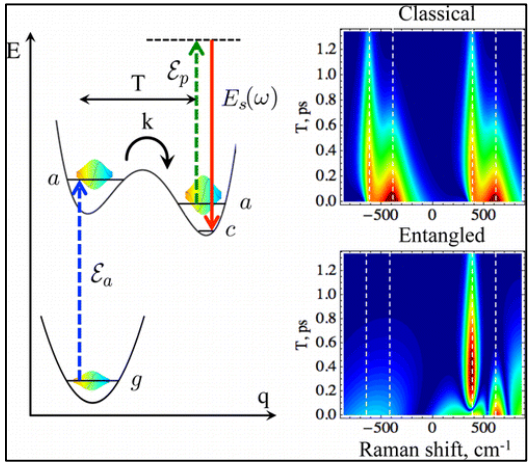
- Opportunities for chemical sciences to advance QIS
  - Design and create tunable qubits
  - Develop probes such as nonlinear, ultrafast x-ray spectroscopies of quantum phenomena
  - Contribute understanding of fundamental principles of quantum phenomena, ultimately leading to 'quantum control'
- Opportunities to exploit QIS for chemical sciences:
  - Quantum sensing of chemical processes (e.g., coherence in photosynthesis)
  - Quantum computing ("Chemistry is quantum computing's killer app" C&E News (Oct 30, 2017)



Ab initio design of molecular magnets – Tb(phthalocyanine)$_2$
(Barnes, Mayhall, Park, Economou)



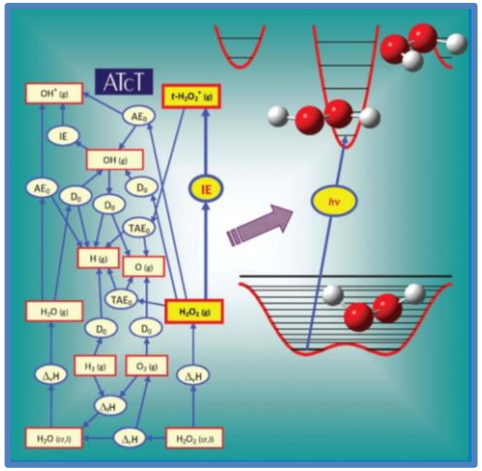
JACS 134, 12430, 2012
(Kobr, Gardner, Smeigh, Dyar, Karlen, Carmieli, Wasielewski)



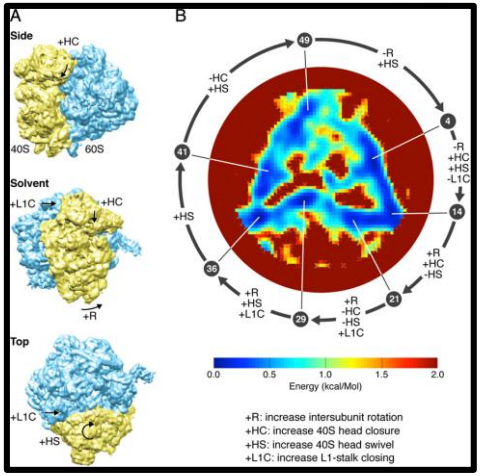
JPC Lett, *5*, 2843, 2014
(Dorfman, Schlawin, Mukamel)

Opportunities in Data Science for Knowledge Discovery

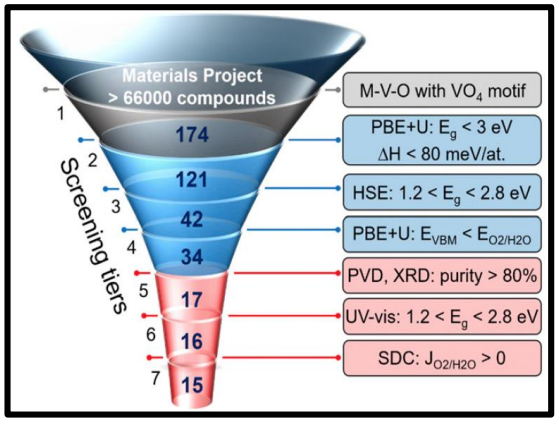
- Recognition of data science needs
  - CSR workshop identified the need to move beyond prediction to develop understanding that can constrain data models
  - Catalysis BRN identify coupled data science, theory and experiment as a priority research direction: “caution is warranted when data science methods are applied without sufficient regard for the underlying scientific basis”
- Emergence of powerful data analytic tools



J. Phys. Chem. A **121**, 8799, 2017
(Changala, Nguyen, Baraban, Ellison, Stanton, Bross, Ruscic)



PNAS 49, 17492, 2014
Dashti, Schwander, Langlois, Fung, Li, Hosseinizadeh, Liao, Pallesen, Sharma, Stupina, Simon, Dinman, Frank, Ourmazd)

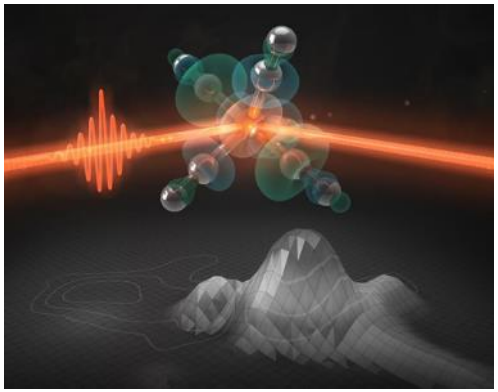


PNAS 2017
(Yan, Yu, Suram, Zhou, Shinde, Newhouse, Chen, Li, K. Persson, Gregoire, Neaton)

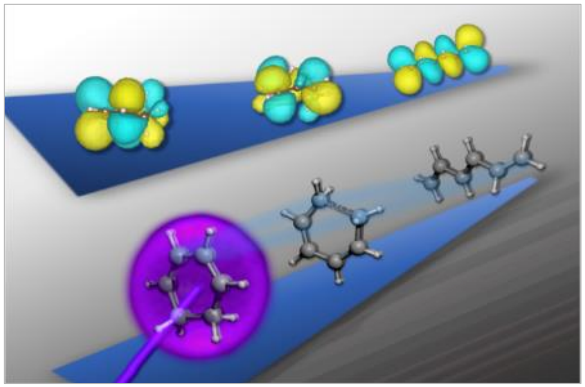
Comments/Questions?

Backup

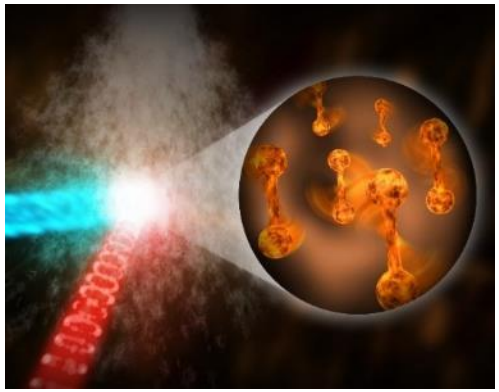
Ultrafast Chemistry



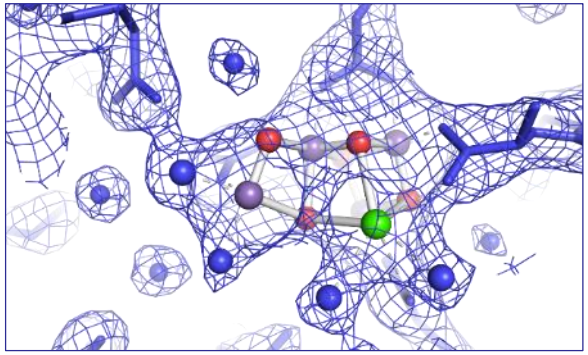
AMOS: *Revealing ultrafast photo-chemistry with x-ray spectroscopy*



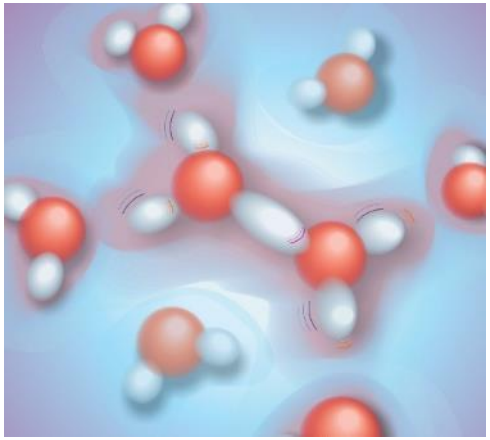
GPCP: *Tracking an electrocyclic reaction with ultrafast x-ray spectroscopy*



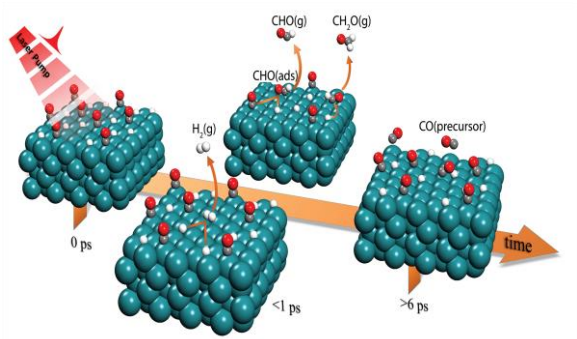
AMOS: *Probing molecular motion with relativistic electrons*



Photosyn: *Taking snapshots of water splitting in photo-synthesis using an x-ray free-electron laser*

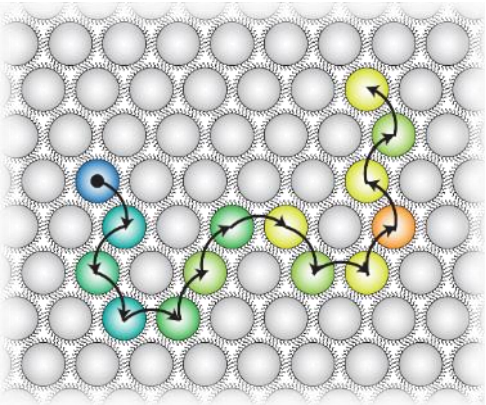


CPIMS: *Resolving strongly mixed intra- and intermolecular character of water vibrations*

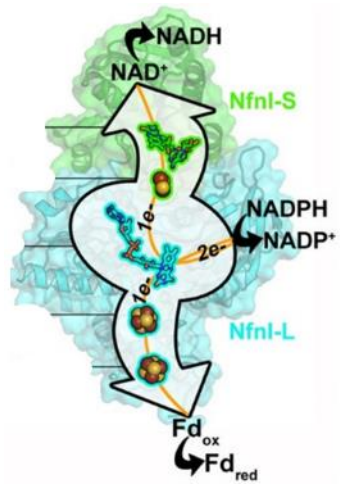


Catalysis: *Elucidating intermediate hydrogenation reaction steps by ultrafast laser temperature jump*

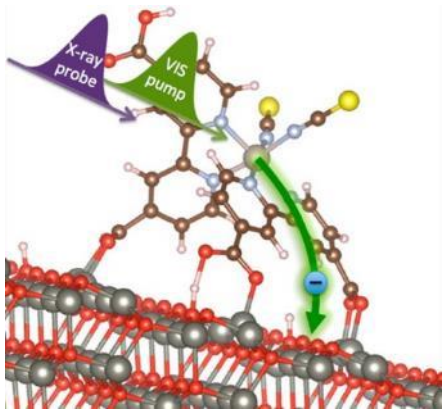
Charge Transport and Reactivity



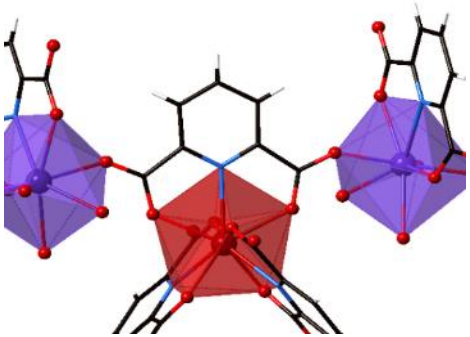
CPIMS: *Quantifying effect of structural and energetic disorder on charge transport*



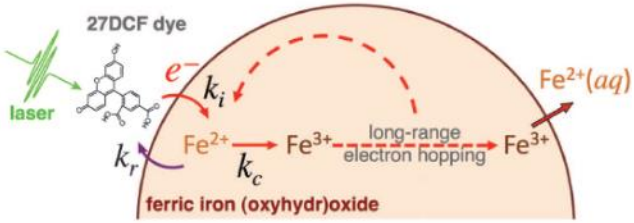
EFRC: *Revealing mechanism of energy conservation by electron bifurcation*



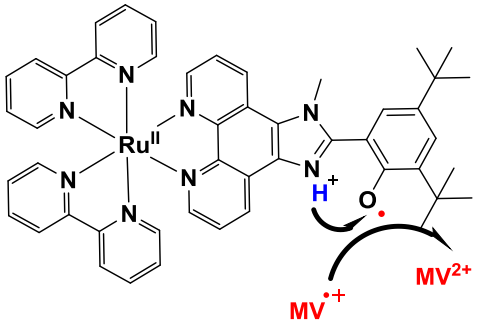
AMOS: *Providing an atomic-scale perspective of ultrafast charge transfer at interfaces*



HEC: *Investigating electron transfer in a plutonium material*

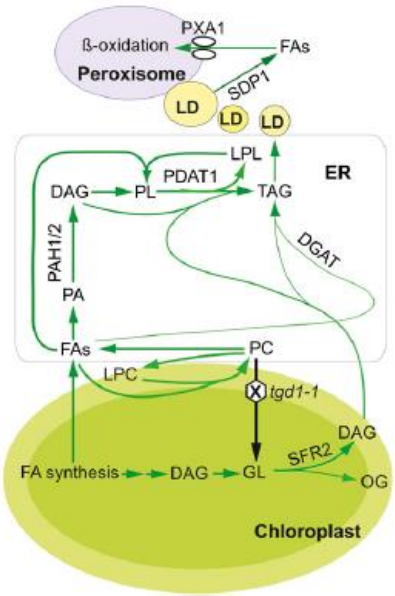


Geosci: *Understanding electron transfer pathways through an iron oxide nanoparticle*

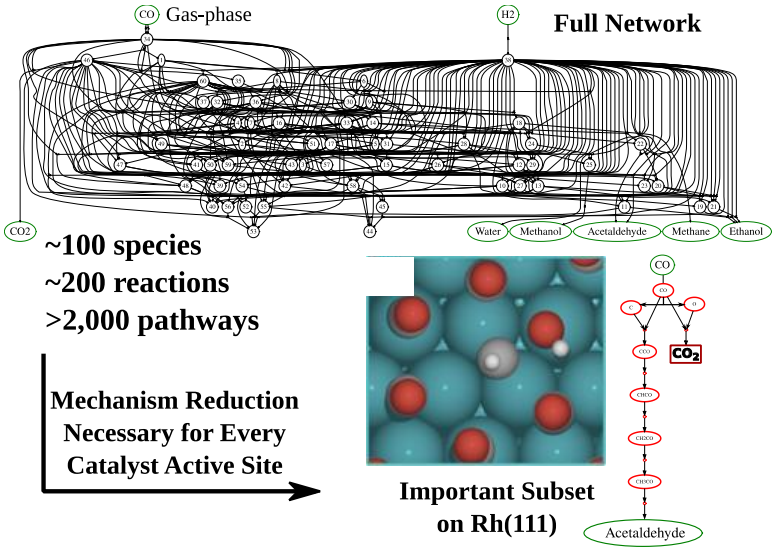


Solar Photo: *Elucidating proton-coupled electron transfer in a linked chromophore-base-phenol complex*

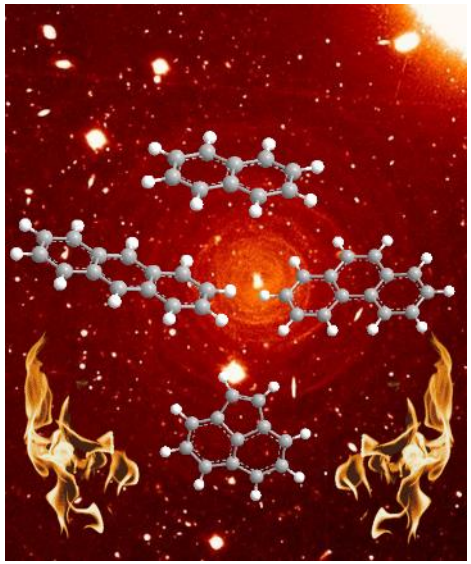
Reactive Pathways in Diverse Environments



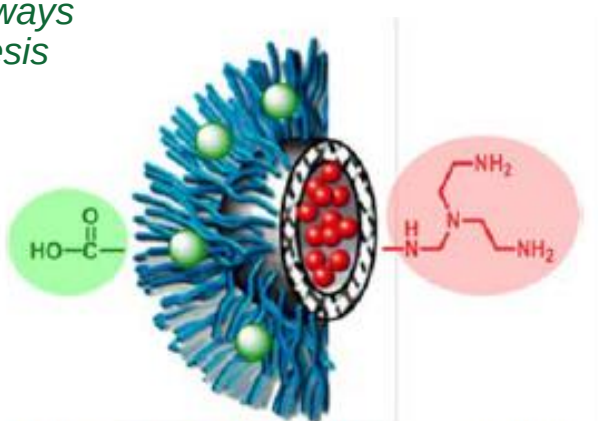
Phys Bio: *Understanding plant metabolic pathways for fatty acid synthesis*



Catalysis: *Addressing surface reaction network complexity using computational and data science tools*

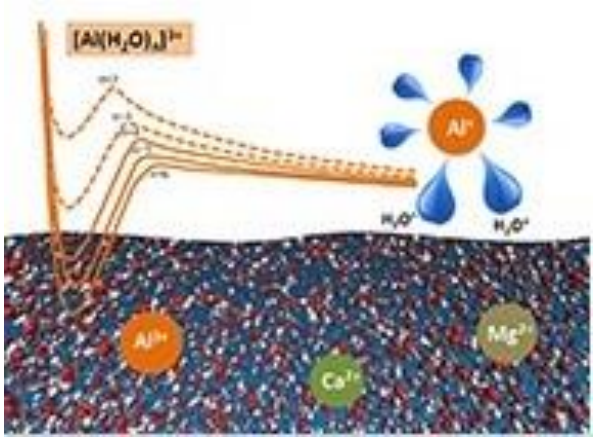


GPCP: *Exploring mechanisms for PAH formation in extreme environments*

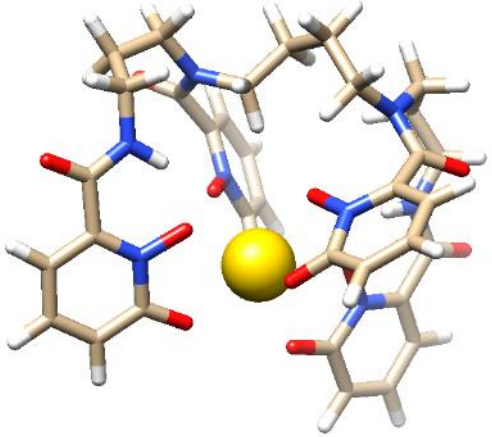


Catalysis: *Developing a strategy to allow a wide variety of tandem reactions that involve incompatible catalytic transformations*

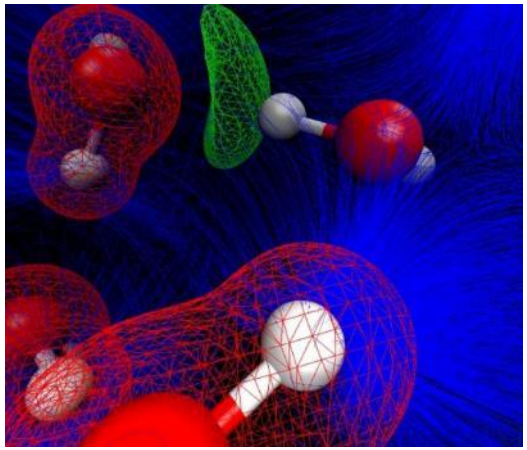
Chemistry in Aqueous Environments



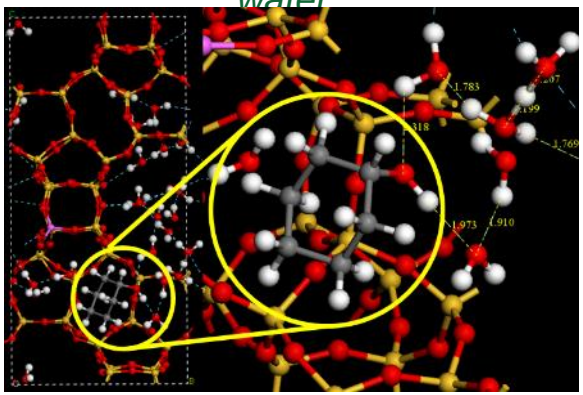
CPIMS: *Stabilization mechanism of multi-charged metal cations in water*



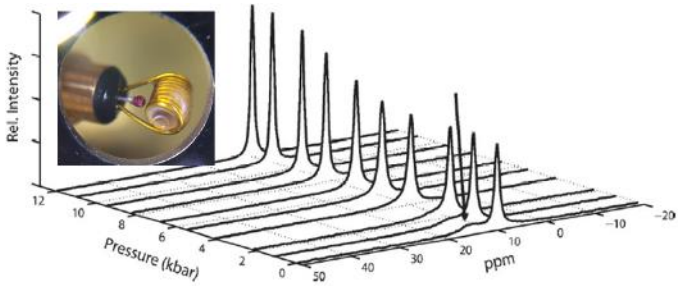
HEC: *Chelating and stabilizing tetravalent Berkelium in aqueous solution*



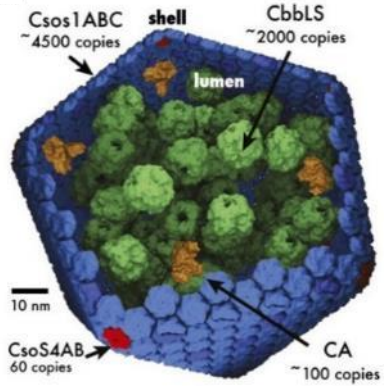
CPIMS: *Understanding how local electric fields affect water*



Catalysis: *Enhancing the catalytic activity of hydronium ions via constraints*



Geosci: *Determining pressure dependence of polyborate species in aqueous solution*



Phys Bio & Photosyn: *Understanding protein-enclosed aqueous environments for CO_2 reduction and other chemistries*