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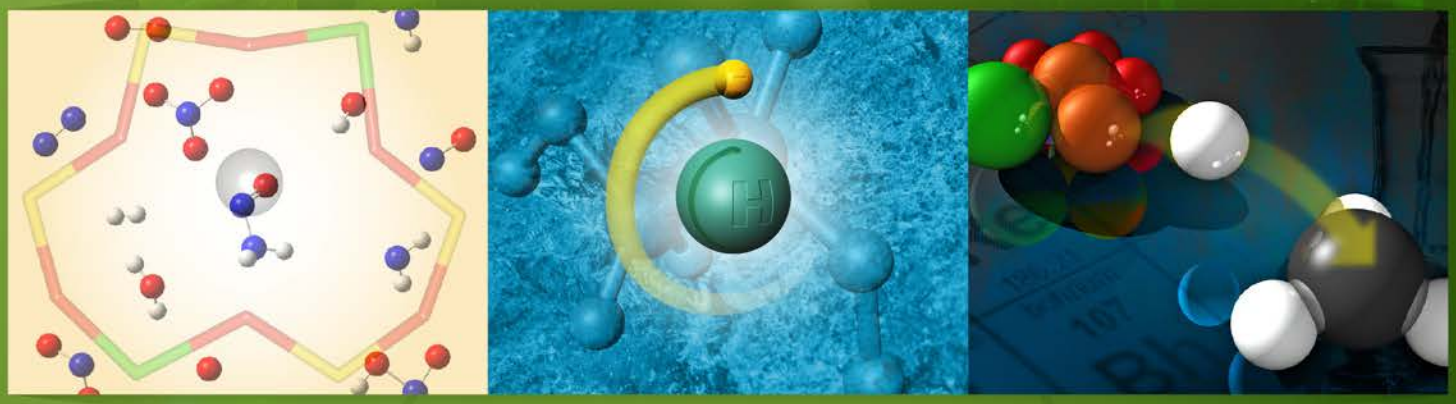
An EMSL Science Theme
Advisory Panel Workshop Report

Opportunities and Challenges

Computation and Modeling of Solvent Mediated Interfacial Processes

Computation and Modelling Focus



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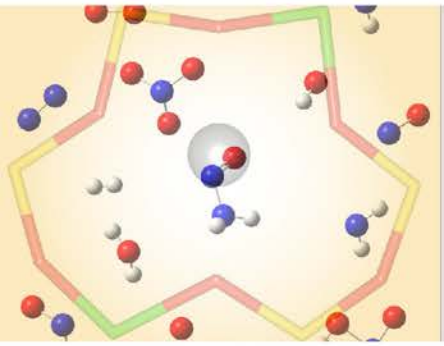
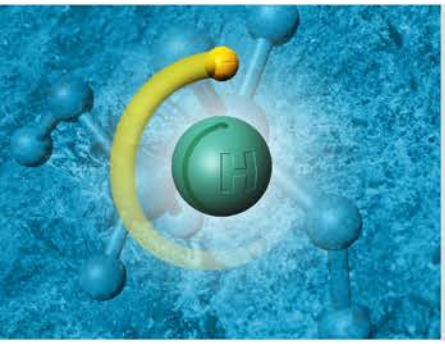


Efficient computational tools are needed for accelerated configurational sampling to account for the state of a catalytic material in realistic environments. Figure courtesy of Professor William Schneider, University of Notre Dame.



Hydrogen production through steam reforming biomass-derived compounds is an economically feasible and environmentally benign way to efficiently use renewable energy resources. A recent study combined experimental and theoretical approaches to compare the hydrogen yield achieved by several metal catalysts used for steam reforming ethylene glycol.

Methanogenic archaea produce more than 90 percent of Earth's atmospheric methane, totaling more than 1 billion tons of methane per year globally. A new study settles a longstanding debate on how this important fuel and powerful greenhouse gas is generated.

High-performance computing available at EMSL is used to develop new multiscale modeling approaches, which enable quantitative linkage between fundamental molecular understanding and predictive simulations at larger scales (biological organisms, communities and ecosystems, aquifers, watersheds, and regional to global climate).

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Opportunities and Challenges: Computation and Modeling of Solvent Mediated Interfacial Processes

An EMSL Science Theme Advisory Panel Workshop Report: Computation and Modelling Focus

Workshop Dates: September 16, 2015

Prepared for the U.S. Department of Energy's Office of Biological and Environmental Research under Contract DE-AC05-76RL01830

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Richland, Washington 99352

Acronyms and Abbreviations

AIMD	Ab Initio Molecular Dynamics
ACS	American Chemical Society
AMBER	Assisted Model Building with Energy Refinement molecular simulation program
APS	American Physical Society
BER	Office of Biological and Environmental Research
CCSD(T)	A version of coupled cluster theory including triple excitations
CHARMM	Chemistry at HARvard Macromolecular Mechanics code
CP2K	An open source molecular dynamics code
DFT	Density Functional Theory
DFTB	Density Functional Tight Binding
DOE	U.S. Department of Energy
EMSL	Environmental Molecular Sciences Laboratory
EMP	Energy Materials and Processes
GROMACS	Molecular dynamics software package
HF	Hartree Fock
LAMMPS	Large-scale Atomic/Molecular Massively Parallel [molecular dynamics] Simulator
MD	molecular dynamics
MSC	Molecular Science Computing
MyEMSL	EMSL data management system to provide data to users
NMR	nuclear magnetic resonance
NWChem	EMSL developed Open Source High-Performance Computational Chemistry Code
PNNL	Pacific Northwest National Laboratory
QMC	Quantum Monte Carlo
QM/QM	Hybrid computation scheme for large systems linking two quantum mechanical codes
ReaxFF	Reactive force field used for molecular dynamics simulations
SciDAC	Scientific Discovery through Advanced Computing
STAP	Science Theme Advisory Panel
XAS	X-ray Adsorption Spectroscopy

Contents

Contents

1.0 Introduction

The report summarizes the discussion and recommendations of a Science Theme Advisory Panel (STAP) focusing on computation and modeling related to solvent mediated interfacial processes. This topic is relevant to all of the science themes at EMSL, the Environmental Molecular Sciences Laboratory; however, the challenges are critical to achieving the decadal objective of the Energy Materials and Processes (EMP) Science Theme to advance understanding of solvent mediated interfacial processes. STAPs made up of leaders in the research community provide input to EMSL regarding areas of science where EMSL can significantly enhance scientific progress, types of capabilities needed to advance that science over the next decade, and the best ways to engage these capabilities to make progress. This lively and productive STAP workshop had much enthusiastic discussion among nine formal STAP members representing nine different institutions, four invited PNNL experts and three EMSL domain experts. Don Baer, EMP Science Theme Lead and Julia Rice, EMSL Science Advisory Committee member from IBM were the STAP organizers.

During FY2016 the EMP science theme will transition to Molecular Transformations. Although aspects of the science theme will shift the issues and recommendations identified regarding computation and modeling in this report, especially those related to the decadal goal dealing with advancing understanding of solvent mediated interfacial processes, remain highly important and equally applicable to the revised science theme as well as the other science themes in EMSL.

EMSL is a national Biological and Environmental Research (BER) U.S. Department of Energy (DOE) user facility with an objective to accelerate scientific innovation for DOE by:

- focusing science on critical problems,
- providing forefront enabling capabilities,
- assembling teams of staff and users with essential expertise to address challenges, and
- marketing these results and capabilities for immediate impact.

Starting in 2012, EMSL initiated a process of realigning and refocusing Science Themes with updated priorities of BER, DOE, and with societal needs. Today EMSL has four BER-aligned Science Themes to focus its scientific resources and user program on the discovery of molecular-scale solutions to pressing challenges in biological, environmental, and energy research:

- Biosystem Dynamics and Design
- Atmospheric Aerosol Systems
- Terrestrial and Subsurface Ecosystems
- Energy Materials and Processes

Energy Materials and Processes was identified as one of the EMSL science themes because sustained economic progress depends on secure, reliable, and affordable energy supplies. Energy and environmental issues related to energy are central to BER and DOE missions. New energy technologies are necessary to address three great challenges: 1) the danger to political and economic **security; 2)** the risk to the global environment from **climate change;** and **3)** the lack of access by the world's poor to the modern energy services needed for **economic advancement.** Because of the need there are many research and technology development activities underway around the world.

The strategic goal of EMP is to develop a sufficient understanding of the dynamic and emergent processes that occur at solvent-mediated interfaces to predict the transformation mechanisms and physical and chemical properties needed for new catalysts for degrading biomass and upgrading of bio-produced fuels and renewable chemicals, and relevant chemical conversion processes. Solvent-mediated interfacial processes are also critical to addressing components of other EMSL

science themes such as aerosol formation and aging, subsurface mineral-solute interactions, and metabolite transport in biological systems.

Phenomena of importance to EMP include charge and mass transport, physical and chemical phase transformations, and catalytic reactions especially those that occur at solid/liquid and solid/gas interfaces. Predictive understanding will be facilitated by linking experimental measurements of interfacial processes and materials properties in response to the process/environmental conditions that impact them with atomic- molecular- and meso-scale models that can be used to guide efficient design of new systems for sustainable energy.

EMSL currently has significant and growing user and research activity in catalytic processes including upgrading of bioproducts, energy conversion and energy storage materials, such as batteries and fuel cells. To optimize impact, we are focusing initial attention in two important areas:

- Optimizing catalytic processes to enhance the production and quality of biofuels and renewable chemicals
- Providing a predictive understanding of the molecular processes needed to design advanced energy conversion and storage.

2015 STAP Focus and Charge

Computation and modeling were identified, both in the first 2014 STAP focused on EMP and an earlier STAP focused on catalysis, as critical components for success in optimizing catalysts, understanding molecular processes at interfaces in energy storage and more generally obtaining predictive knowledge of solvent mediated interfacial processes important in several areas of EMSL. There are many types of needs: enhanced ability of codes to predict properties which enables the design of new materials and systems and can guide the design of high impact experiments; there is a need to speed the link between modeling and experiment, enabling rapid data analysis to rapidly guide to follow-on experiments; there needs to be a hierarchy of computational codes working and connected across multiple length and time scales with different degrees of fidelity.

We specifically asked the STAP to provide recommendations in the following areas:

- What **next generation high priority codes** (and related computational capabilities) are needed to significantly advance modeling related to catalysis, energy storage and other solvent/mediated processes?
    - Which software tools exist in the community and can be leveraged, and which should be developed as part of NWChem or other EMSL-based software?
    - What are the key hardware needs (e.g., large memory, fast-access disk, large node counts, accelerators) to support execution of these codes?
- What should be included in the suite **of hierarchical codes** with appropriate levels of fidelity and complexity to tackle solvent mediated processes, catalysis and energy storage?
    - What tools or frameworks should be developed to facilitate linkage of codes across a hierarchy of scales?
- What actions should we take to significantly increase the **visibility, accessibility and application** of NWChem in the catalysis community?
    - What level of workflow guidance and creation of easy to use interfaces are needed to facilitate the ability of the catalysis and battery community to access EMSL codes.

As expected the STAP discussion provided a wide range of inputs related to enhancing the impact and value of EMSL.

2.0 Workshop Structure and Recommendations

2.1 Structure

The workshop agenda (appendix A) was constructed to encourage researchers with a variety of expertise to provide input on the desired topics. The elements of the workshop included:

Overview presentations:

- EMSL science themes with a particular focus on EMP
- Feedback from previous STAPS
- EMSL Computational Strategy
- NWChem Status and Development Strategy

Participant Input

- Short presentations by STAP members on important needs or directions. *These short presentations served to identify the interests and expertise of the STAP members and provide an initial foundation for more detailed discussion.*
- Four Breakout discussion sessions followed by reports and group discussion:
  1) Software/Hardware Needs
  2) Models of the Solid/Liquid Interface
  3) Modeling needs at multiple scales and transfer across scales
  4) Experiment-Theory Integration

  Details of the breakout session questions, the participants and the reports are included in section 2.3
- Overall discussion, identification of opportunities and needs
- At the end of the workshop each participant was given the opportunity to give the important overall impressions and recommendations. These have been captured in the general recommendations below.

2.2 General Recommendations

The energetic discussion at the STAP workshop was energetic and diverse. The following themes emerged as important for the development of computation that would impact the EMP and each of the other science themes in EMSL.

Nature and Types of Needs

- **Solvent effects are critical** to understanding sorption, reaction and transport processes on surfaces and at interfaces relevant to catalysis, batteries, aerosol formation and aging, subsurface processes and other systems relevant to DOE and BER. Without considering solvent impacts reaction processes, phase transformation and binding energy calculations can be both quantitatively and qualitatively wrong.
- Current **computational codes** dealing with solvent mediated interfacial reactions **can (need to) be advanced/extended** in important ways that include: specific consideration of **entropy** effects; including the impactions and variations due to the **dynamics** of system elements; and expanded ability to systematically and quantitatively explore impacts of variations in **configuration** space.
  - Current calculations often provide useful relatively information when entropy and enthalpy are highly correlated. Need to sample entropy and configuration space.

  - System dynamics can play an important role in reactivity as well as understand the impact of experimental measurements. It may seem obvious that a molecule changes in response to the surface, but the surface also responds in the presence of a molecule.
- The complex systems of importance to BER/DOE require modeling at **multiple time** and **spatial scales**. There are modeling needs at multiple scales and an ability to transfer relevant/important information across scales.
  - There is need for a suite of codes covering multiple length and time scales with well-defined workflows that can link them (cross scales).
    - Accurate and efficient atomic and molecular level codes can provide parameters that make biological codes smarter and establish a more rigorous foundation for larger scale codes.
    - Need additional physics codes to complement molecular chemistry codes.
  - Need to facilitate linking of lower cost models to some of the higher-level models available in NWChem.
  - Need case studies or other methods that highlight how to perform low-cost screening calculations to identify where more accurate calculation may have the highest value.
- Different types of tools are needed to engage and support a **shifting/evolving user/developer community**. There is both a need for advanced state of the art codes that will be used by computational **experts** and codes that can be appropriately run and validated by **non-experts** including experimentalists seeking to plan experiments and understand data.
  - There are many domains for which state of the art codes should be used only by researchers with considerable experience or under the guidance of such experts. As noted above, advances in code and computation capabilities are needed to adequately address critical problems. We should not pretend that many of these codes can be appropriately applied to complex problems by those without considerable experience.
  - However, it is also increasingly relevant and important for experimentalists to have access to models related to experimental data and important for users of specialized data (e.g., UV/Vis, NMR, XAS, neutron scattering, microscopies, etc.) to be able to appropriately model their systems and experiments. In many cases the expertise of a 'professional' modeler is not needed. It is also necessary for a non-expert model user to have information and some understanding the limitations and boundary conditions for which "routine" codes are valid.
    - The development or sensible default parameters in common useful codes and "pipelines" for system set up would be very useful.
  - With the many types of codes that are available and which may be applied, having a series of "benchmark" calculations would be a service to the community allowing experts and non-experts to explore the limitations, relative accuracy and errors produced using various parameters or approaches.

Unique or distinguishing opportunities for EMSL Computation

NWChem provides a very strong platform to build upon. It can be the foundation needed for advancing codes, a way to provide an accurate foundation and reliable parameters for more empirical codes and a source for user friendly codes for non-expert users. The open source nature, the outstanding performance on a variety of systems and free availability position it uniquely. It can be optimized, packaged and integrated in ways to provide a distinctive role in addressing the complex problems important to DOE and BER.

- Develop seamless integration of multiple types/levels of models
  - Periodic, cluster, embedded and more
  - Enable sensitivity testing, data sharing and high level benchmarking

    - Provide well-grounded physical and chemical parameters for higher level models (help bio and other larger scale codes be 'smarter')
    - Improved QM/MM and QM/QM codes are an important opportunity space
    - Benchmarking data sets, identification and enhanced ease of use in specific application domains (case studies)
    - Integrating NWChem with established and widely used classical molecular dynamics codes like Amber and LAMMPS
- Modeling of Spectroscopies/Experimental data
    - Provide a uniform umbrella of novice/expert tools for computing a broad range of spectroscopies
- Develop advanced methods for structure and configuration space searching
    - Ab initio molecular dynamics (AIMD), accelerated searching configuration space, advanced transition state searching, variational transition state theory (VTST), probability mass function (PMF), metadynamics, basin hopping, etc.
    - In an easily usable/accessible environment
- Take advantage of next generation computing
    - Optimize codes for advanced computers, expanding accuracy and speed increasing the complexity of problems that can be addressed

Barriers, Challenges, Needs and Opportunities

- Need to make integration of NWChem and other codes easier to facilitate both codes advances and multi-scale modeling
- Need to improve accessibility, connectivity, automated or guided workflow, ease of use
    - Smart default values
    - Sensible default parameters, pipelines and automated workflows
    - Easy to use library interface
    - Need infrastructure enabling components to plug into NWChem
- Need to enhance visibility and "branding" of NWChem and overall EMSL computation capabilities
    - Expert and non-expert user
    - Tutorials
    - Case studies and benchmark calculations
    - Domain specific training and examples
- Code needs
    - Add capabilities to NWChem that extend beyond what is available in many codes (some as described above and additional descriptions in the Hardware/Software breakout session report)
        - Green's function approaches
        - Need periodic (planewave) response for spectroscopies to complement molecular capabilities
    - Continued development and code maintenance
        - NWChem (molecular & periodic) needs to be robust for "standard" calculations and non-expert use
            - Energies, gradients, transition states, ab initio molecular dynamics
        - Maintain consistent institutional support
        - Link fast/cheap calculation to enable better use of accurate costly codes
        - Maintain/enhance speed on new generation computers
    - Spread development effort
        - Quick prototyping workshops

- Developer workshops with focused application groups

2.3 Breakout Groups: Topics, Questions, Reports and Participants

Each break out session was to keep in mind the overall questions presented to STAP (STAP charge in Section 1), some general breakout questions and specific questions relevant to each breakout group and specific questions for the breakout topic, including anything they thought important. The reports are recorded with minimum changes in an attempt to reflect the thoughts needs and recommendations of the group.

- General Questions:
  - How can EMSL best address the needs or opportunities associated with the topic?
  - What should we do and what should we let others do?
  - What will most impact scientific impact?
  - Short- and long-term objectives?
- Discussion leader is to encourage and coordinate discussion.
- Reporter assists the discussion leader, keeping some type of summary of the main conclusions.
  - Leader or reporter reports back to whole group.

Breakout #1: Software/Hardware Needs

Initial Questions, Issues or Input from Previous STAPs

- *"The EMSL Computational Plan should encompass plans for NWChem/other user software, hardware and associated infrastructure/energy needs/upgrades, data management (e.g., MyEMSL) and data storage."*
- *Next generation computer*
- *Software needs, limitations (we cannot do everything)*
- *Computational capabilities should extend in both spatial and temporal regimes for better linkages between experiment and modeling.*

Group Report

Hardware Needs:

1. Quantum codes (NWChem) have provided an "upper bound" on computing needs at EMSL.
   a. This is a good strategy
2. Possible ways to support/co-exist with other science themes and satisfy BER sponsor
   a. Different partitions for type of computer use to accommodate less intensive codes
   b. Thick and thin nodes…

Software Needs:

1. Complete software rewrites are not cost effective
2. NWChem is an "island"
   a. Needs more interoperability
   b. Not visible on user interfaces
   c. Needs to bridge to other capabilities in the open source community
3. Need infrastructure components to plug into NWChem

    a. Expose interfaces
4. Develop a quick prototype to plug into open source visualizer to serve as a template
5. Developer meetings
    a. For discussion and implementation of code
    b. Involve graduate students
    c. Coding focused ("hackathons") instead of presentations (as in Seattle workshop)
6. User group meetings
    a. Outreach (ACS, APS meetings?)
    b. Identify application groups
    c. Target domains
7. NWChem (molecular & periodic) needs to be robust for "standard" calculations
    a. Energies, gradients, transition states, ab initio molecular dynamics
8. Absolutely need a robust PAW implementation + potentials in the NWChem planewave module
9. Absolutely need periodic (planewave) response for spectroscopies to complement molecular capabilities
    a. NWChem will be unique if this is accomplished.
    b. Unique opportunity for NWChem in theoretical spectroscopies
10. Integrate xclib library. xclib has a broad developer base.
    a. Can coexist with our nwxc lib? Needs discussion
11. Dispersion models (self-consistent approach, Tkachenko-Scheffler)
12. Interface NWChem planewave module to GW/BSE implementations
    a. Implementations from the Rehr group
    b. Ocean
    c. ETSF codes
13. Periodic Gaussian basis implementation
    a. Opportunities for periodic HF, DFT and higher-order correlation approaches
    b. Connection to QMC codes
14. Move NWChem beyond what is available in some areas
    a. Green's function approaches, etc.
15. Other needed development areas
    a. Traversing long time scales
    b. Thermodynamic sampling
    c. Tackling dynamics processes that occur on different time scales
    d. Time resolved transition states
    e. Transient spectroscopies
    f. Free energy sampling
    g. Phonon effects on spectra (UV/Vis, XAS, NMR)

Participants

John Rehr – discussion leader
Axel Kohlmeyer - reporter
Doug Baxter
Simone Raugei
Adolfy Hoisie
Jeff Hammond
Karol Kowalski

Breakout #2: Models of S/L interface - range of applications

Initial Questions, Issues or Input from Previous STAPs

- *Ten year goal: Solvent-mediated Interfacial Chemistry*
- *Relevant to other EMSL science themes*
- *Status of current codes? Current limitations? What needs to be developed?*

Group report - Summary of Discussion

What are the needs #1

- Cut the bulk, add solvent, and watch the system change.
  - The truncated homogeneous bulk is not the S/L interface.
  - What is the structure of the electrochemical interface?
  - Where do the electrons go? What is the charge?
  - How is a molecule stabilized by the surface and the solvent?

What are the needs #2

- Well characterized systems to study and do what UHV people do.
- Make connection to experimental studies of the buried interface. Do they exist?
- Better calculation of solvation energies, dielectric response
- Automated tools to calculate work functions and the complexity associated with polar systems.

What are the needs #3

- Continuum above the solid? Beyond Poisson Boltzmann? “Joint DFT” RISM-like.
- Automated, rational transition from cluster to periodic systems. Are they self-consistent?
- Automated sensitivity decisions.
- Answer the question: how sensitive are results to the choices that we make.

Where will we make the most impact?

- Do simple things that help people now
- NWCHEM has an identity problem.
- Web site of structure
- Web based tutorial
- YouTube channel showing how to get started
- Graphical user interface?
- Can we take other interfaces and plug into NWCHEM?
- Reduced models are useful: DFTB, ReaxFF, NNDO, …
- Issue: It costs the life a graduate student to parameterize. Make something robust and easier!
- Develop consistency between frameworks: molecular, continuum, transport, coarse grained, …

Participants

Chris Cramer, discussion leader
Greg Schenter, reporter
Bill Cannon
Thomas Bligaard
John Keith
Susannah Scott
Bill Schneider

Johannes Lercher
Niri Govind
Amity Anderson
Simone Raugei

Breakout #3: Modeling needs at multiple scales and transfer across scales

Initial Questions, Challenges or Starting input from previous STAP

- A hierarchy is needed having computation codes covering multiple length and time scales, well defined workflows, and more physics codes.
- Facilitate the linking of lower cost methods to some of the higher-level models also available in NWChem
- Highlight how to perform low-cost screening calculations to identify where more accurate calculations may have highest value

Group Report

Hierarchical Code Needs

NWChem is well recognized for efficient, large scale CCSD(T). That should be the core of multiscale developments in the code.

The current QM/MM interface is very useful capability. However:

- Need to improve the user interface: It would be great if the code could directly read the most common MM topologies (Amber, Gromacs, Charmm, etc.).
- Need for a more accurate and physically sound electrostatic coupling between the QM and MM subsystems (e.g., multigrid schemes)

We foresee huge opportunities QM/QM schemes: different levels of embedding, from correlated wavefunction approaches, to DFT, to MM, to coarse grained, to potential embedding, and possible up to continuum model. To be competitive there is the need to include statistical sampling (MD and Monte Carlo).

Many challenging issues should be addressed and solved (long-term commitment):

- What kind of information to transfer between scales
- How to transfer mass and energy between scales
- How to transfer the time information between scales

It will be also critical to understand errors (accuracies) and reach consistency (wavefunction, density, multipoles, etc.) between the different representations (scales).

Concerning the MM representation, we do **not** see any reason to go into the polarizable force field arena.

NWChem for preliminary, low-cost screening calculations

We do not anticipate that NWChem will be a code of choice for large throughput screening. **However, improved implementations of linear scaling approaches in NWChem (density fitting and local approximation) would make the code more competitive for use over the next decade.** Here are some additional suggestions:

- Probably need to build interface for fast sampling approaches (for instance, LAMMPS for molecular dynamics)
- Probably there will be the need of more sophisticated and user friendly interfaces, which go beyond Python, for controlling the flow of data.
- Need to be able multiple calculations at the same time with little data exchange between them (something similar to the 'farming' schemes in CP2K).
- Need to have fast initialization times (currently too much time required for initialization). [2]

Participants

John Keith, discussion leader
Simone Raugei, reporter
Chris Cramer
Axel Kohlmeyer
Bill Cannon
Greg Schenter
Adolfy Hoisie

Breakout #4: Experiment-Theory Integration

Initial Questions, Challenges or Starting input from previous STAP

- *The EMSL computational Plan should explain how the computational capabilities will be fully integrated with the experimental/observational capabilities*
- *Computational capabilities should extend in both spatial and temporal regimes for better linkages between experiment and modeling.*

Group Report

Experiment-Theory integration
Agree that it is desirable, but what is it?
It is already happening to a large extent
Talked about interaction paradigms
desire healthy back-and-forth interaction, development of hypotheses, insights
theory provides conceptual framework, not just numbers
little value in just computing what has already been measured
Materials design "prediction" paradigm has probably been oversold
Design problem in general factorial complex, Synthesis problem even more so
community should learn from order parameter approaches

Tools for interfacing theory/experiment
Electronic, vibrational, magnetic spectroscopies
Microscopies, energy loss

Scattering
Transient methods
Lots of tools exist
Some not as widely/easily available as they should be
Exciting new tools to develop
Need “novice” and “expert” user modes
Put tools in the hands of the users

What are the opportunities to distinguish NWChem and other EMSL Computation Capabilities?

1. Seamless integration of models
    a. periodic, cluster, embedded
    b. enables sensitivity testing, data sharing, high level benchmarking
2. Spectroscopies
    a. uniform umbrella of novice/expert tools for computing a broad range of spectroscopies
3. Advanced methods for structure searching
    a. AIMD, accelerated searching, advanced transition state searching, VTST, PMF, metadynamics
    b. In a easily usable environment
4. Takes advantage of next generation computing

Participants

Susannah Scott, discussion leader
Bill Schneider, reporter
Thomas Bligaard
John Rehr
Johannes Lercher
Niri Govind
Amity Anderson

3.0 Workshop Agenda

Energy-Catalysis-Computation
EMSL Advisory Panel

EMSL Room 1077

Wednesday, September 16, 2015	
Time	**Topic(s)**
8:15 a.m.	Welcome and Introductions
8:30 a.m.	STAP Charge, Overview of EMSL Science Themes and EMP and feedback from previous STAPs – Don Baer
9:00 a.m.	STAP Members Identification of Important Directions
10:20 a.m.	Break
10:30 a.m.	EMSL Computational Strategy – Karol Kowalski
10:55 a.m.	NW Chem Status and Development Directions – Niri Govind
11:20 a.m.	Introduction of Breakout Sessions and Discussion of Objectives
11:30 a.m.	Pick up lunch and head to breakout sessions in Room 1075
11:40 a.m.	Small Breakout Session 1 • Group 1 Discussion: Software/Hardware Needs (Meet in 1077) • Group 2 Discussion: Models of S/L interface - range of applications (Meet in 1019)
1:00 p.m.	Report back from break session 1 and discussion (meet in 1077)
1:30 p.m.	Introduction to Break out session 2 • Group 1 Modeling needs at multiple scale and transfer across scales (meet in 1077) • Group 2 Experiment-Theory Integration (meet in 1019)
2:50 p.m.	Break
3:00 p.m.	Report back from break session 2 (meet in 1077)
3:30 p.m.	Discussion of opportunities and needs
4:20 p.m.	Synthesis of high level recommendations
5:15 p.m.	Adjourn

4.0 Workshop Attendees

Energy Materials and Processes Science Theme Advisory Panel (STAP) Workshop Participants

STAP Workshop Organizers
Donald Baer, PNNL – Co-Chair
Julia Rice, IBM – Co-Chair*

STAP Members
Thomas Bligaard,
SLAC

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University of Minnesota

Jeff Hammond,
Intel

John Keith,
University of Pittsburgh

Axel Kohlmeyer,
Temple University

Johannes Lercher,
PNNL

Bill Schneider,
University of Notre Dame

Susannah Scott,
University of California at Santa Barbara

*Unable to attend

PNNL Expert Participants

Bill Cannon
Adolfy Hoisie
Simone Raugei
Greg Schenter

EMSL Subject Matter Experts

Amity Anderson
Karol Kowalski
Niri Govind