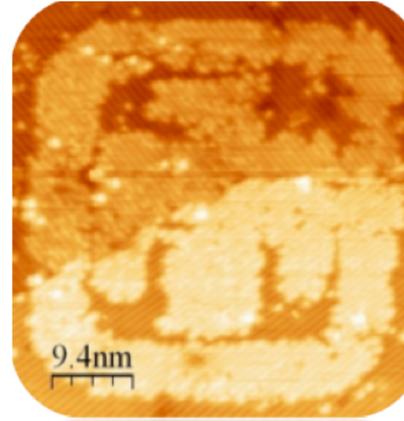
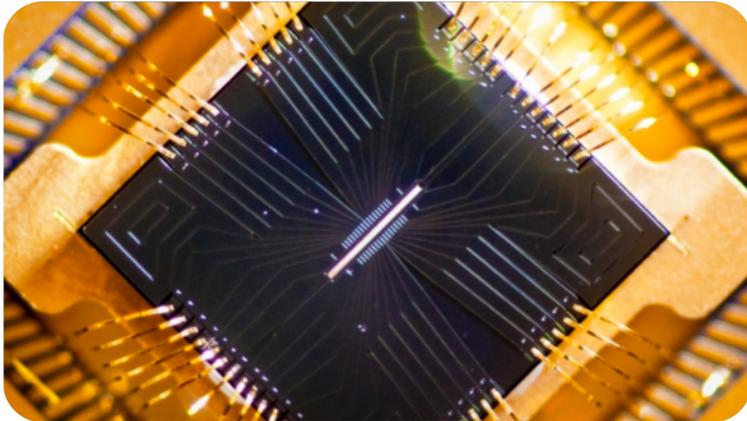


Exceptional service in the national interest



Robust quantum simulation for near-term realizable quantum hardware

Richard P. Muller, Robin Blume-Kohout, Jonathan E.

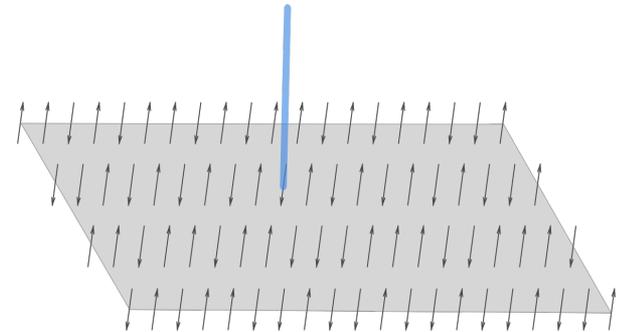
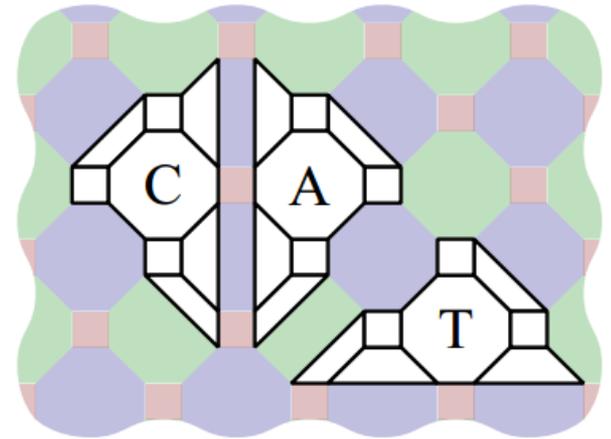
Moussa, Andrew J. Landahl



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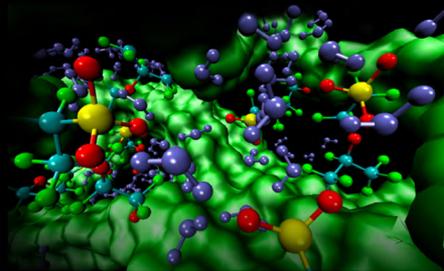
Near-term promise of quantum

- Long-term promise of quantum is well-known
 - FT-QEC enabling large circuits simulating factoring, unstructured search, etc.
 - DOE-relevant problems: optimization, graph properties, quantum simulation
- What can we do in the near term (10 years)?
 - It is likely we will have some special purpose quantum hardware that can establish and manipulate quantum states in this time frame.
 - Probably not enough qubits to perform QEC **and** an algorithm
 - What algorithms can we identify?



Simulation is Central to ASCR & DOE Sandia National Laboratories

SEPTEMBER 2012
FROM QUANTA TO THE CONTINUUM:
OPPORTUNITIES FOR **MESOSCALE SCIENCE**
A REPORT FOR THE BASIC ENERGY
SCIENCES ADVISORY COMMITTEE
MESOSCALE SCIENCE SUBCOMMITTEE



A Workshop to Identify Research Needs and Impacts in
Predictive Simulation for Internal Combustion Engines (PreSICE)

Sponsored by the Office of Basic Energy Sciences, Office of Science and the Vehicle Technologies
Program, Office of Energy Efficiency and Renewable Energy, U.S. Department of Energy

Thursday, March 3, 2011

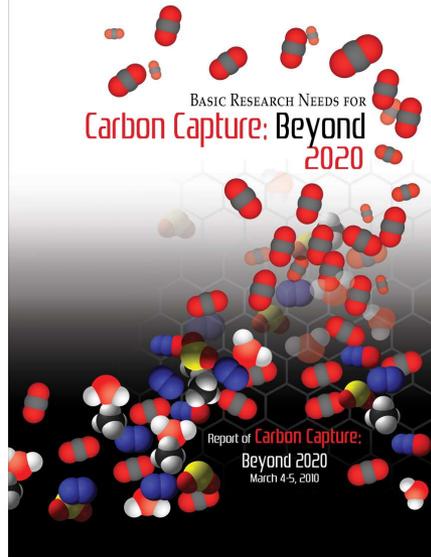


U.S. DEPARTMENT OF **ENERGY** Office of Science

U.S. DEPARTMENT OF **ENERGY** Energy Efficiency & Renewable Energy

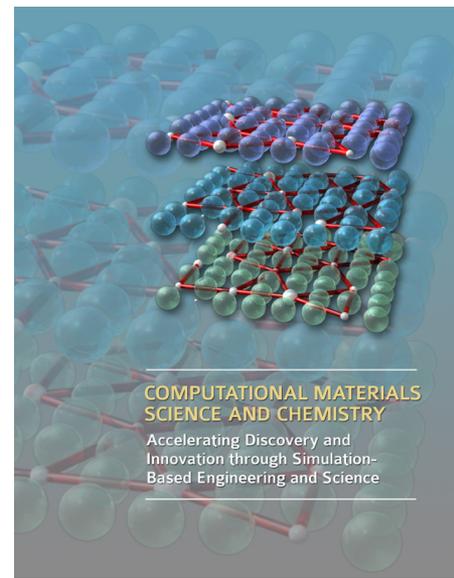
BASIC RESEARCH NEEDS FOR
Carbon Capture: Beyond 2020

Report of **Carbon Capture:
Beyond 2020**
March 4-5, 2010



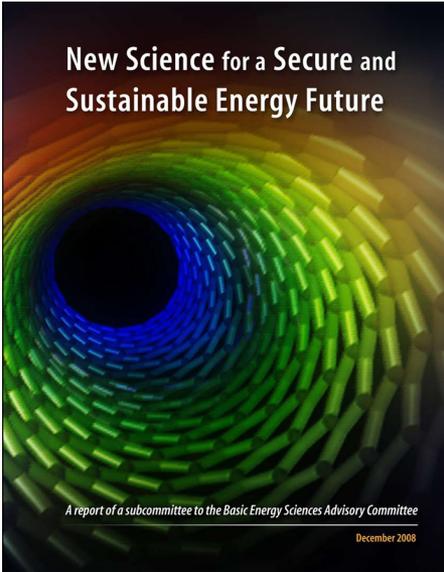
**COMPUTATIONAL MATERIALS
SCIENCE AND CHEMISTRY**

Accelerating Discovery and
Innovation through Simulation-
Based Engineering and Science



**New Science for a Secure and
Sustainable Energy Future**

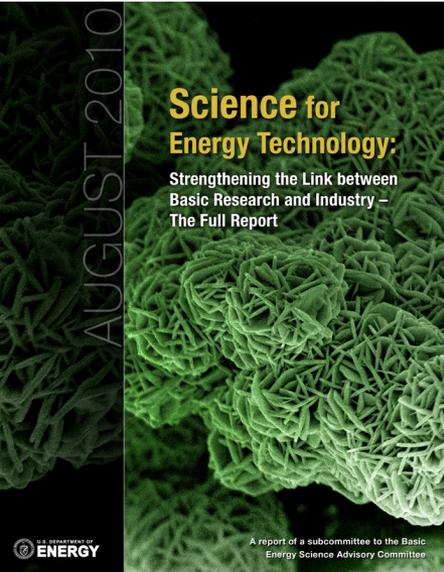
A report of a subcommittee to the Basic Energy Sciences Advisory Committee
December 2008



**Science for
Energy Technology:**

Strengthening the Link between
Basic Research and Industry –
The Full Report

AUGUST 2010

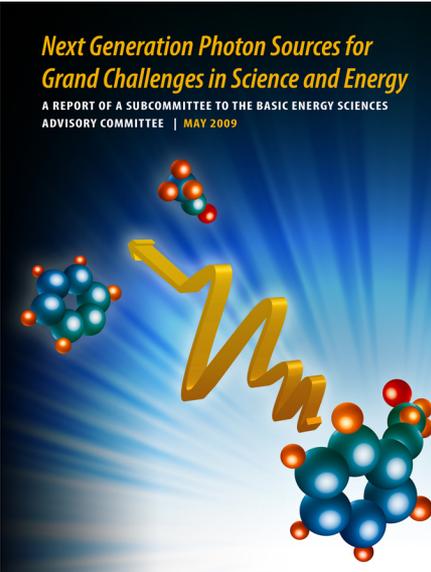


U.S. DEPARTMENT OF **ENERGY**

A report of a subcommittee to the Basic
Energy Science Advisory Committee

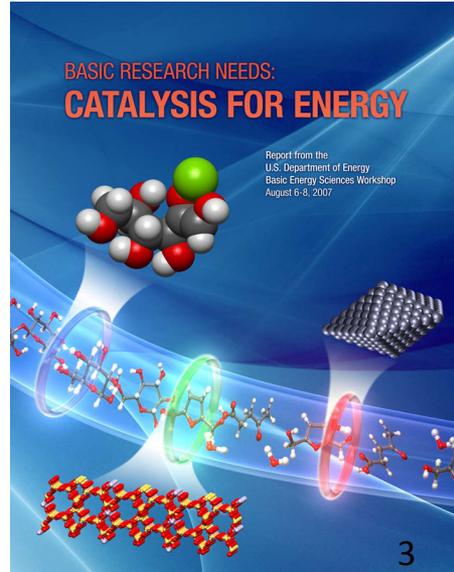
**Next Generation Photon Sources for
Grand Challenges in Science and Energy**

A REPORT OF A SUBCOMMITTEE TO THE BASIC ENERGY SCIENCES
ADVISORY COMMITTEE | MAY 2009



BASIC RESEARCH NEEDS:
CATALYSIS FOR ENERGY

Report from the
U.S. Department of Energy
Basic Energy Sciences Workshop
August 6-8, 2007

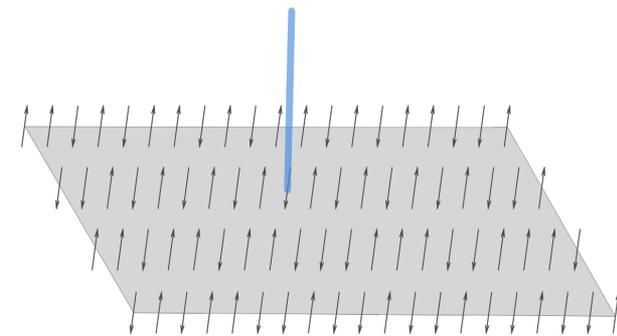
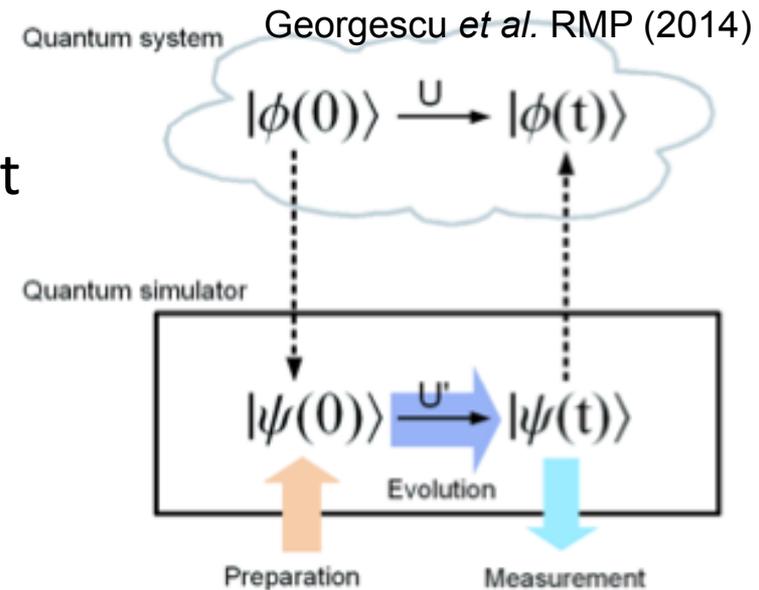


Robust quantum simulations

- Robustness
 - Since we can't afford FT-QEC, we need algorithms that are somehow robust to noise, disorder, decoherence.
- Potential robust algorithms
 - Analogue simulation of quantum systems
 - Device noise mimics simulation noise
 - Shallow quantum oracles
 - Variational eigensolver by Peruzzo et al from quantum chemistry
 - Minimize the build-up of noise with shallow circuits
 - Dissipative quantum processes
 - Perform operations with stable fixed points that are insensitive to noise in the distant past

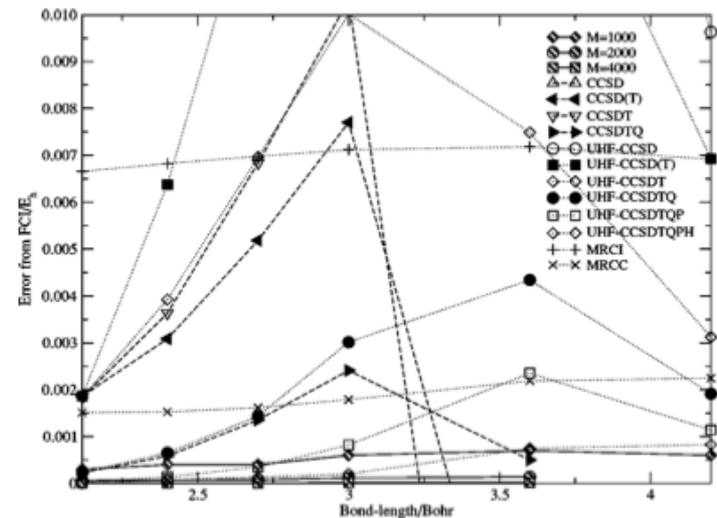
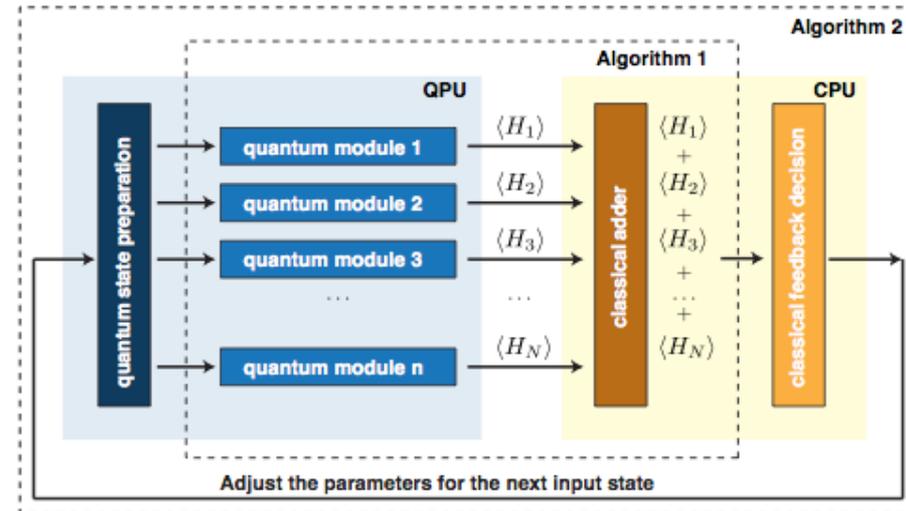
Analogue simulation of quantum systems

- Arrange qubits so that their Hamiltonian closely approximates that of the quantum system of interest.
- Useful for lattice properties of materials
 - e.g. Does Fermi-Hubbard model with X parameters superconduct?
- Robust because of assumed similarity between device noise and system noise
 - Need to understand how well noise models map between analogues



Variational quantum eigensolver

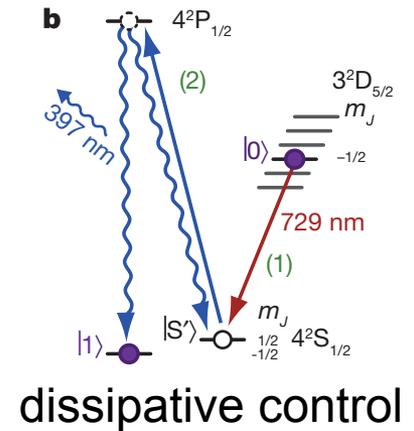
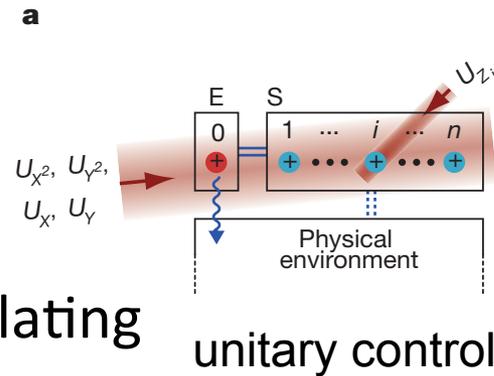
- Example of shallow oracle
- Prepare and measure quantum states based on few classical parameters that are varied and optimized using classical means
- Need to identify wave functions where polynomial optimization results in something computationally useful
- UCC very promising
 - Size consistency and variational are not exclusive, and may both be required for materials design
 - Is UCC unique?



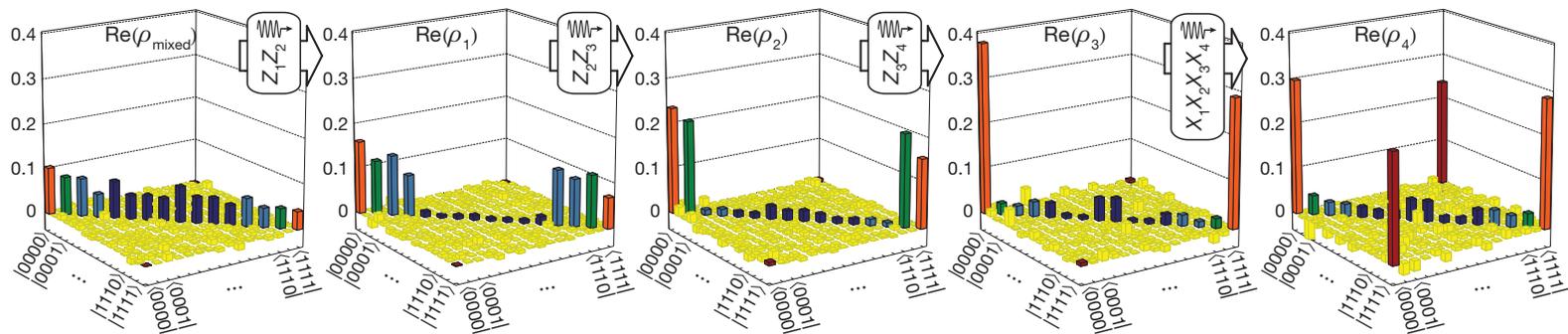
Chan et al., JCP (2004)

Dissipative quantum processes

- Overwhelm unintentional loss with engineered loss
- Noise *perturbs* the steady state from the ideal instead of accumulating *drift over time* of a state from the ideal
- Natural platform for open system dynamics
- “Easy” to engineer quantum correlations, hard to protect quantum information:



Barreiro et al., Nature (2011)



Path forward

- Office of Science mission to a large degree involves materials simulation
- Robust simulation promises
 - Quantum speedup without overhead of QEC
 - Clearest application to DOE-relevant problems
- Some of this problem space may be explored in the very near term via quantum **emulation**
 - Direct simulation of quantum vector states possible for small numbers of qubits
 - Use noise models extracted from GST studies of existing systems (e.g. arXiv 1310.4492)
 - Establish how device space and simulation space noise models map for different types of simulation.
- In-depth partnership with experiment is necessary for validation and continued progress.