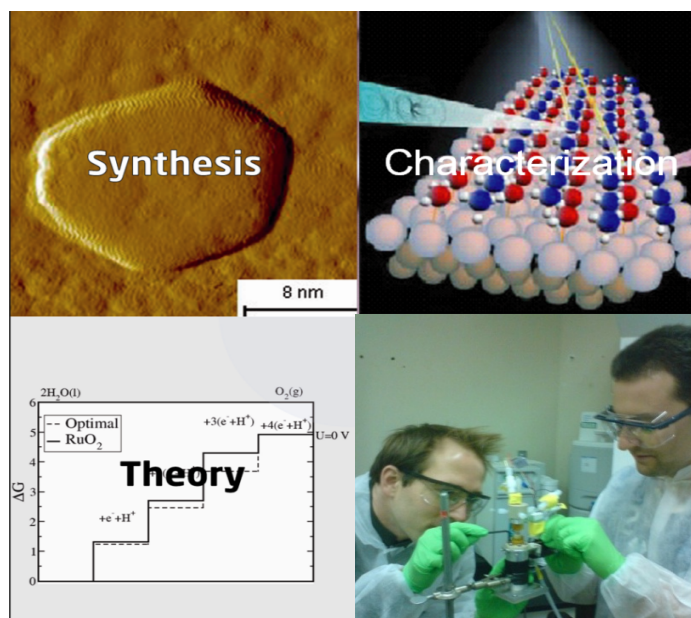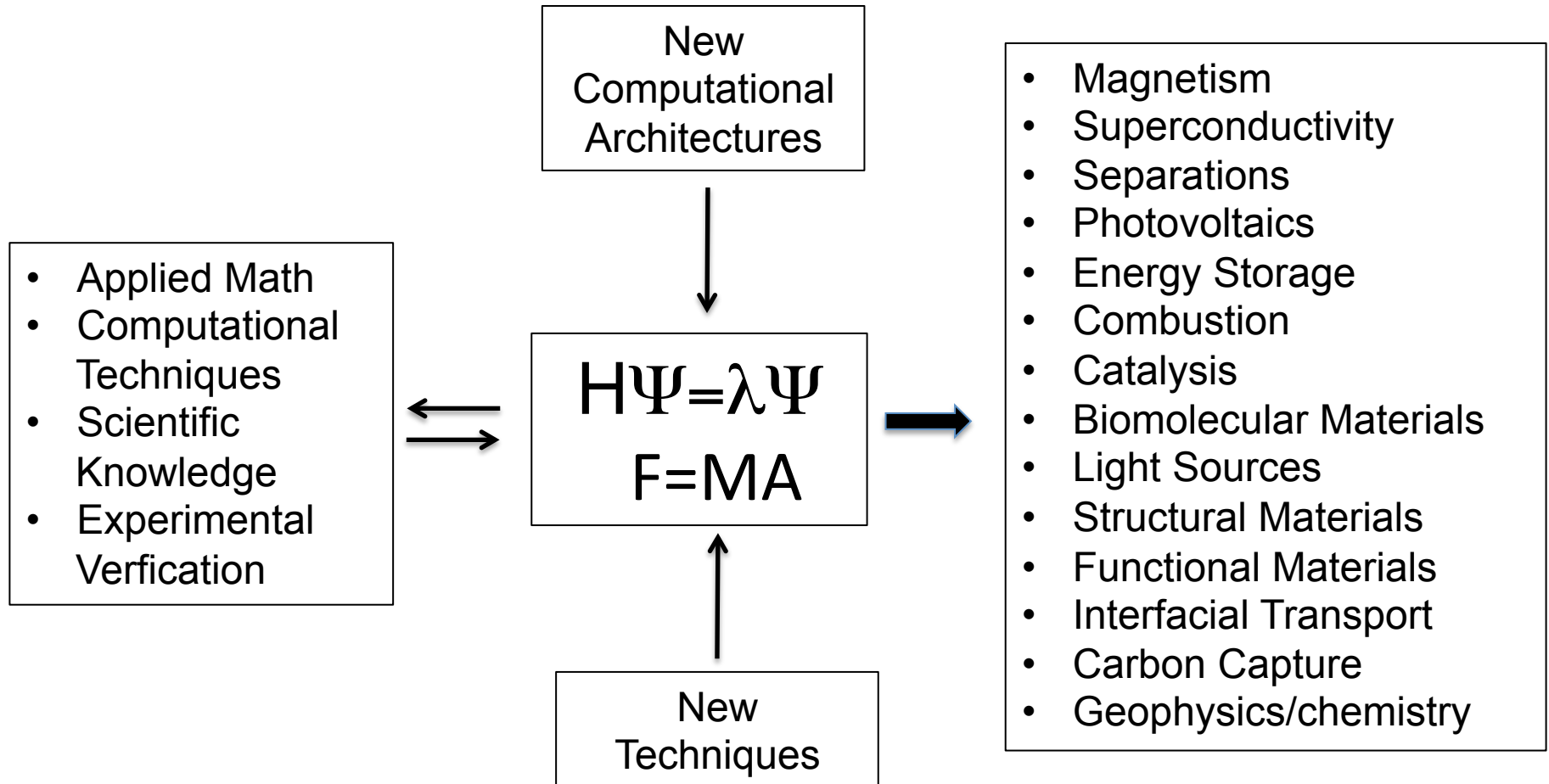# BES SciDAC - 24 July 2013

Mark R Pederson

Theoretical and Computational Chemistry
Basic Energy Sciences
Office of Science, U.S. Department of Energy
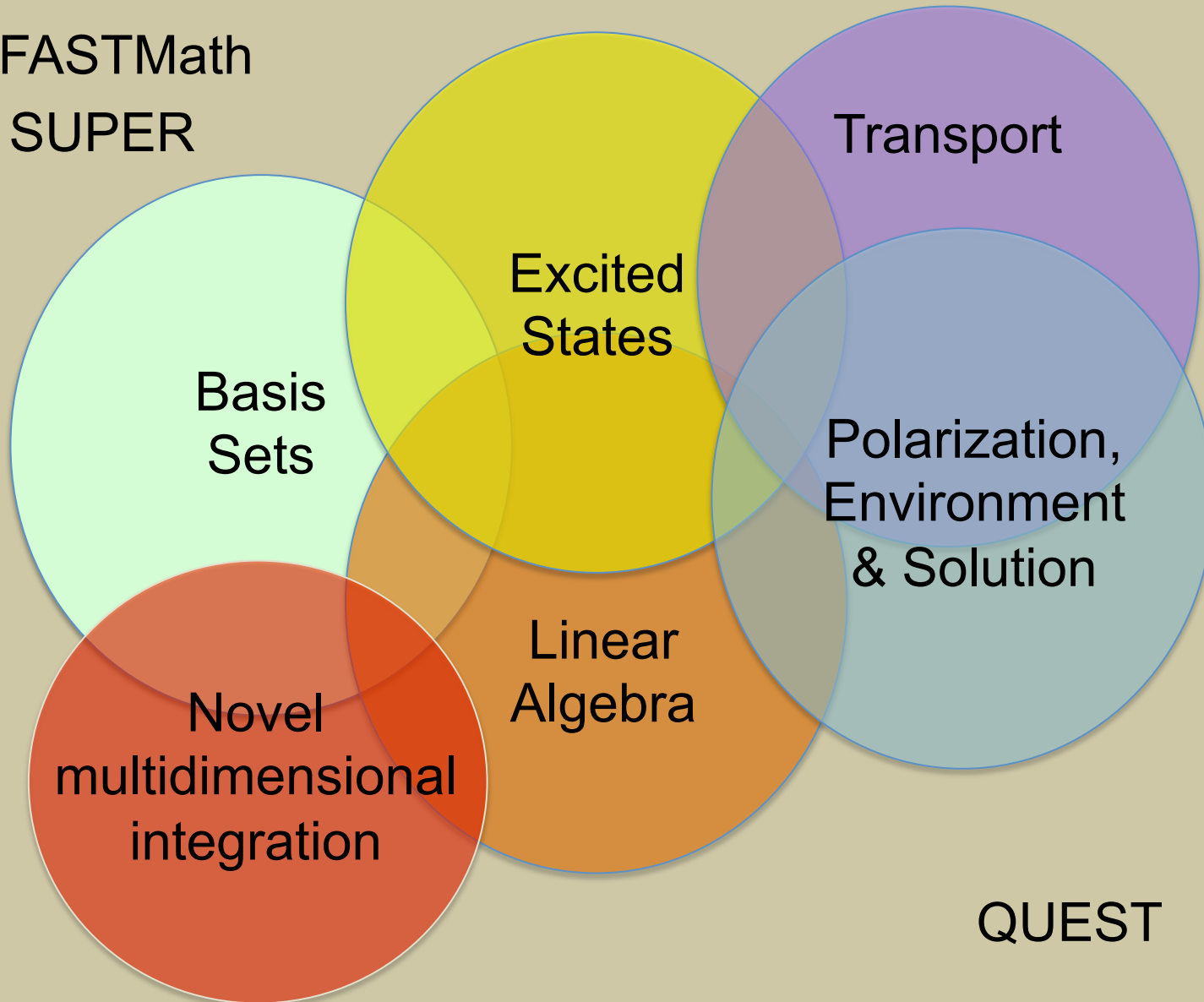

Materials: James Davenport
Chemistry: Mark Pederson

One Need for the BES Predictive Theory and Modeling Mission

New
Computational
Architectures

- Applied Math
- Computational
  Techniques
- Scientific
  Knowledge
- Experimental
  Verfication

$$H\Psi=\lambda\Psi$$
$$F=MA$$

New
Techniques

- Magnetism
- Superconductivity
- Separations
- Photovoltaics
- Energy Storage
- Combustion
- Catalysis
- Biomolecular Materials
- Light Sources
- Structural Materials
- Functional Materials
- Interfacial Transport
- Carbon Capture
- Geophysics/chemistry

BES SciDAC PROJECTS

- *Predictive Computing for Condensed Matter* **(So Hirata, Wed 1:00PM)**

- **Optimizing Superconductor Transport Properties through Large-Scale Simulation (Andreas Glatz / Thu 9:45AM)**

- **Discontinuous methods for massively parallel QMD: Li-ion interface dynamics from first principles (John Pask, Thu 11:00 AM)**

- **Scalable Computational Tools for Discovery and Design: Excited State Phenomena in Energy Materials (Jim Chelikowsky, Thu 1:30PM)**

- *Water, soft matter and reactions in solution: major challenges to microscopic modeling and simulation* **(Roberto Car, Fri 9:00 AM)**

- **Simulating the Generation, Evolution and Fate of Electronic Excitations in Molecular and Nanoscale Materials with First Principles Methods (Martin Head-Gordon, Fri 9:45 AM)**

- **Developing Advanced Methods for Excited State Chemistry in the NWChem Software Suite (Chris Cramer, Fri 11:00AM)**

BES SciDAC TALKS

- **QMC*: Predictive Computing for Condensed Matter* (So Hirata, Wed 1:00PM)**

- **MESH*: Computational studies of vortex dynamics and pinning effects in high-Tc superconductors* (Andreas Glatz / Thu 9:45AM)**

- **MESH*: Discontinuous methods for large-scale quantum molecular dynamics: challenges and outlook* (John Pask, Thu 11:00 AM)**

- **MESH: *Excited States and Spectroscopic Properties of Condensed Matter: Theoretical Developments and Computational Challenges* (Steven Louie, Thu 1:30PM)**

- **PARTICLE: *Water, soft matter and reactions in solution: major challenges to microscopic modeling and simulation* (Roberto Car, Fri 9:00 AM)**

- **PARTICLE: *Very Large Scale Linear Algebra for Bound and Unbound Electronic States: Challenges and Opportunities* (Dan Haxton, Fri 9:45 AM)**

- **PARTICLE: *Charge transfer and charge transport in photoactivated systems: Challenges in modeling chromophore solvation, aggregation, and flexibility* (J. Ilja Siepmann, Fri 11:00AM)**