

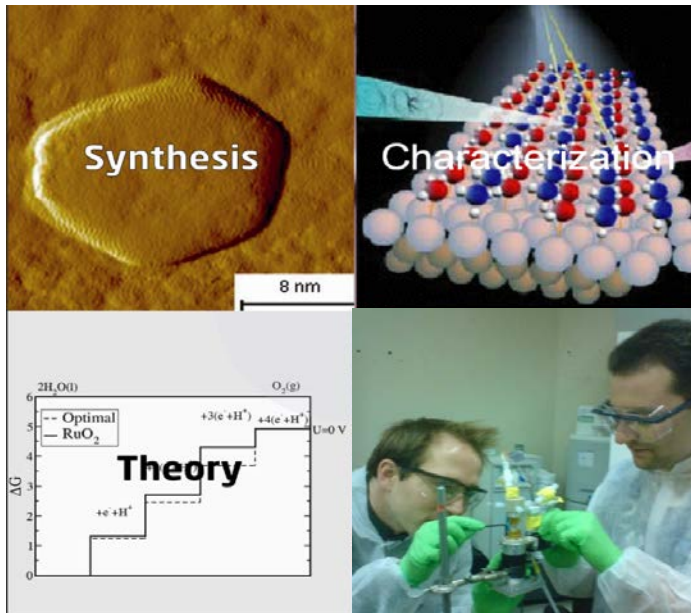
BES SciDAC - 22-24 July 2015

<http://www.orau.gov/scidac3pi2015>

Mark R Pederson

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

Hyatt Regency Bethesda MD



Materials: James Davenport
Chemistry: Mark Pederson

ASCR: Ceren Susut

Office of Basic Energy Sciences

Harriet Kung, Director

Wanda Smith, Administrative Specialist

BES Budget and Planning

Katherine Chen, Financial Management
 Doneira Herbert, Financial Management
 Thomas Russel, Senior Technical Advisor

BES Operations

Kerry Hochberger, Program Support Specialist
 Robin Hayes, Program Manager
 Natalia Melcer, Program Manager
 Katie Runkles, Program Analyst / BESAC*
 Andy Schwartz, Senior Technical Advisor for EFRCS*

* Basic Energy Sciences Advisory Committee
 * Energy Frontier Research Centers

Materials Sciences and Engineering Division

Linda Horton, Director

Teresa Crockett, Program Analyst
 Vacant, Program Assistant
 Ashley Dyke, Intern

Scientific User Facilities Division

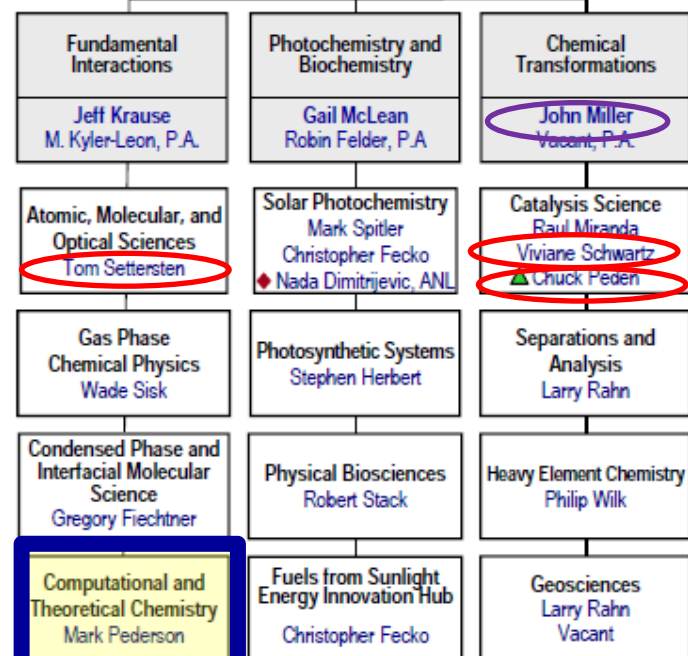
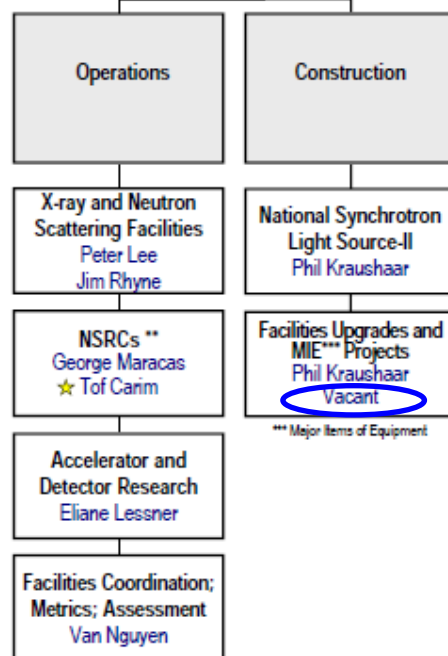
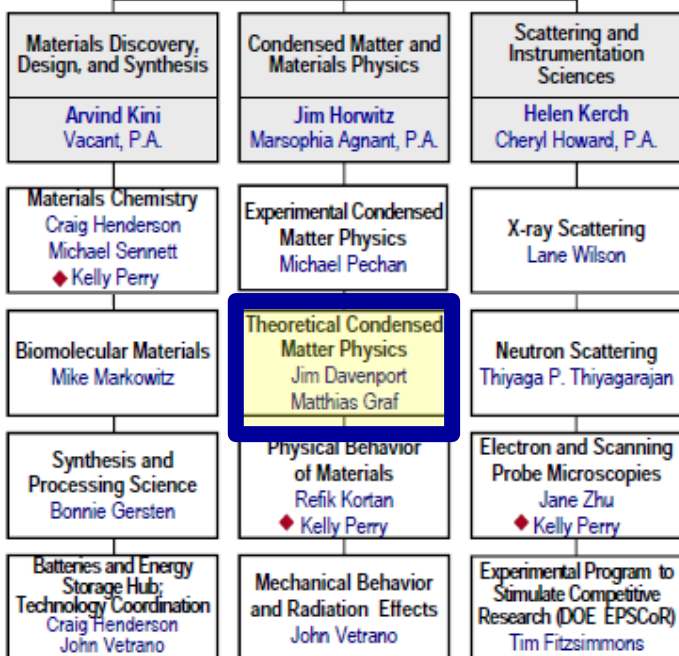
James Murphy, Director

Linda Cerone, Program Support Specialist
 Rocío Meneses, Program Assistant

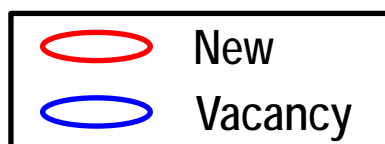
Chemical Sciences, Geosciences, and Biosciences Division

Tanja Pietraß, Director

Diane Marceau, Program Analyst
 Vacant, Program Assistant
 Joshua Haines, Intern



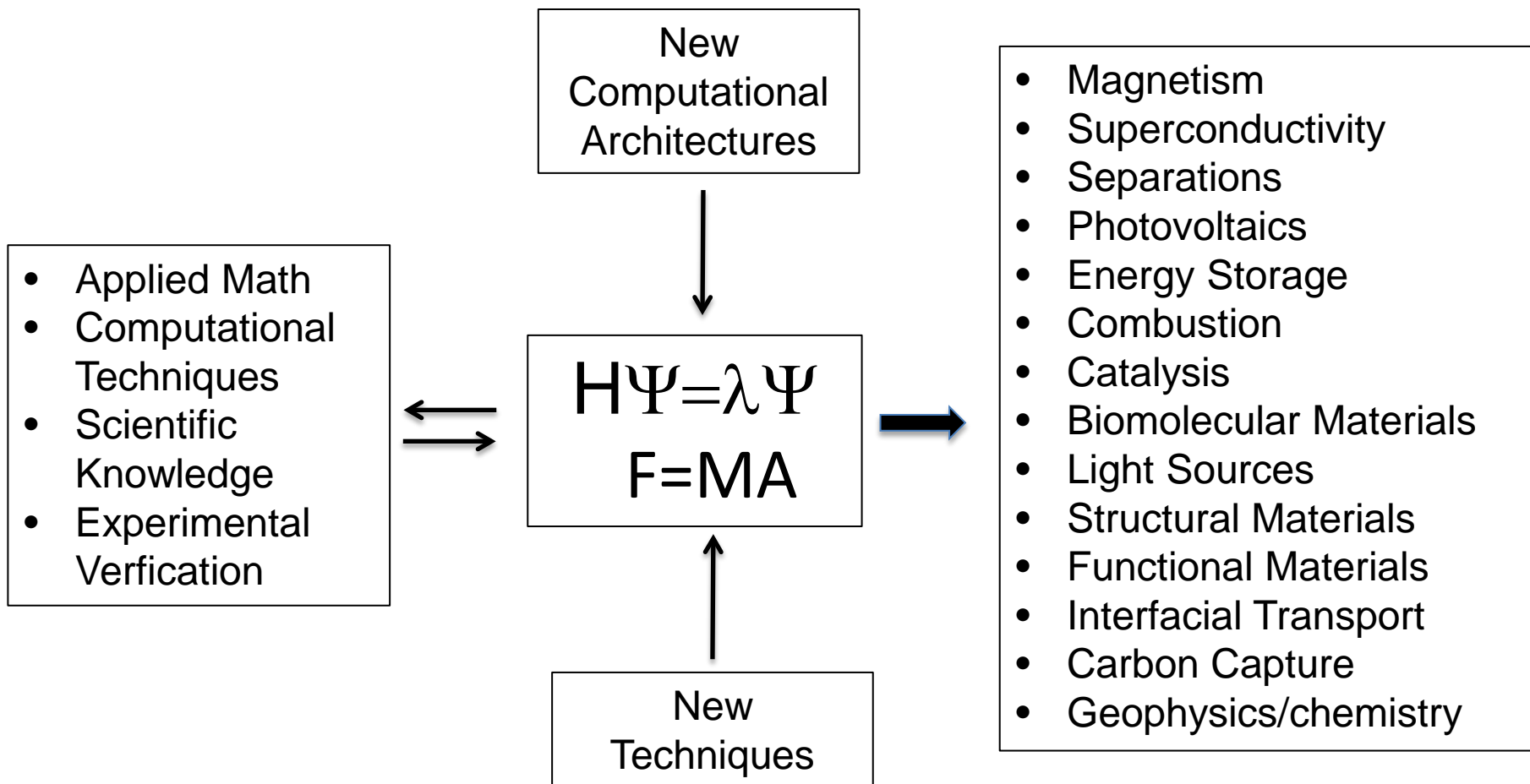
** Nanoscale Science Research Centers



Retiring
 July 2015

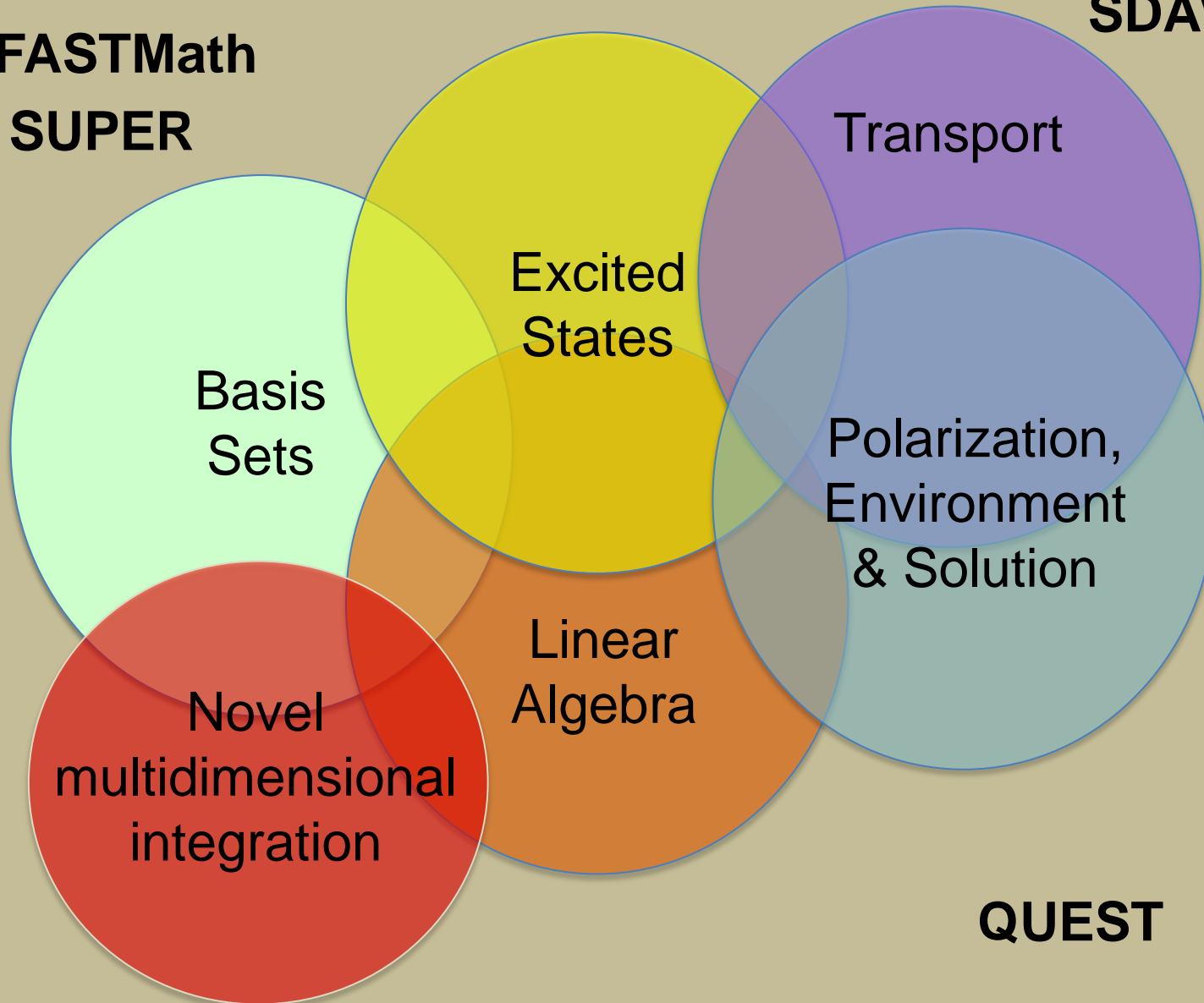
LEGEND
 ★ On detail to OSTP
 ♦ Detailee from DOE Laboratory
 ▲ IPA from BMI/PNNL
 P.A. Program Assistant

One Need for the BES Predictive Theory and Modeling Mission



FASTMath
SUPER

SDAV



QUEST

BES SciDAC PROJECTS

- **Advanced Modeling of *Ions in Solutions*, on Surfaces, and in Biological Environments** (PI: Roberto Car / Speaker: Xifan Wu Wed 3:00 PM)
 - **Optimizing *Superconductor Transport Properties* through Large-Scale Simulation** (PI: Andreas Glatz / Speaker: Andreas Glatz Thu 9:45AM)
 - **Scalable Computational Tools for Discovery and Design: *Excited State Phenomena in Energy Materials*** (PI: Jim Chelikowsky / Speaker Jack Deslippe, Thu 11:00 AM)
 - **Discontinuous *Methods* for *massively parallel* QMD: *Li-ion interface* dynamics from first principles** (PI: John Pask / Speaker: John Pask Thu 2:30 PM)
 - ***Predictive Computing* for Condensed Matter** (PI: So Hirata / Speaker Garnet Chan Thu 3:45PM)
 - **Simulating the Generation, Evolution and Fate of *Electronic Excitations* in Molecular and Nanoscale Materials with First Principles *Methods*** (Martin Head-Gordon / Speaker: Martin Head-Gordon, Fri 9:45 AM)
 - **Developing Advanced *Methods* for *Excited State* Chemistry in the NWChem Software Suite** (PI: Chris Cramer / Speaker: Bert de Jong, Fri 11:00AM)
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