U.S. DEPARTMENT OF ENERGY

# *SciDAC-3 PI Meeting*

## Washington

## July 30, 2014

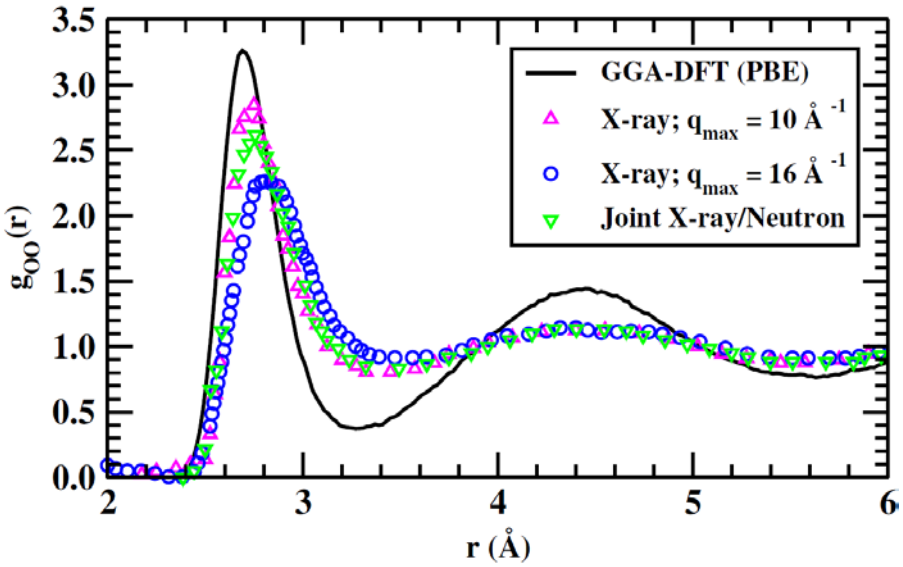
**Jim Davenport**
**with**
**Mark Pederson & Ceren Susut**

# BES/ASCR SciDAC Talks

- Advanced Modeling of Ions in solutions, on Surfaces, and in Biological Environments - Roberto Car
- Scalable Computational Tools for Discovery and Design: Excited State Phenomena in Energy Materials - Jim Chelikowsky
- Developing Advanced Methods for Excited State Chemistry in the NWChem Software Suite - Don Truhlar
- Optimizing Superconductor Transport Properties through Large-Scale Simulations - Andreas Glatz
- Simulating the Generation, Evolution and Fate of Electronic Excitations in Molecular and Nanoscale Materials with First Principles Methods - Martin Head-Gordon
- Predictive Computing for Condensed Matter - Lucas Wagner
- Discontinuous methods for massively parallel QMD: Li-ion interface dynamics from first principles - John Pask

# SciDAC Program – Key Components

- **Advance Science**
  - Projects important to BES
- **Collaborative**
  - Teams with Applied Math and Computer Science PIs
- **Use Leadership Class Machines**
  - Titan, Mira, Edison
- **Materials Science is a full fledged partner**
- **Chemical Sciences had been all along**



# Other Programs in BES

- Predictive Theory and Modeling
- Started the same year – 2012
- 19 Awards, $13 million
- Light weight alloys, TM oxide Catalysis, Photosynthesis, The Materials Project, QMC, others
- BES contribution to the Materials Genome Initiative
- Strategic Plan http://www.nist.gov/mgi/upload/MGI-StrategicPlan-2014.pdf
- White House Blog http://wh.gov/l6rT2

# New Program in Computational Materials Science

- Part of FY 2015 Budget Request to Congress
- $24 million for up to 4 large teams of experts in materials theory, modeling, computation, synthesis, characterization, and processing/fabrication.
- Basic research required to develop and deliver research-oriented software and associated databases for predictive design of functional materials.
- Received $8 million in House Markup and $18 million in the Senate
- Stay tuned

# Connections

- **Funding for BES SciDAC projects is partly in Materials, partly in Chemistry, and partly in ASCR**
- **Reflects the convergence of many of the techniques, algorithms. Advances in one area often lead to advances in another**
- **Other Connections as well**
- **QCD – relevance to hadrons, nuclear structure, nuclear matter**
- **Workshop – Rich Brower & Eduardo Fradkin**
  **Field Theoretic Computer Simulations for Particle Physics and Condensed Matter**
  **http://blogs.bu.edu/ppcm/program/**