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Student Presentations, March 2015
Academic and Professional Background

- PhD in Physics from the University of California at Berkeley
- Worked in industry at AT&T (Bell Labs), Exxon Research and Engineering, XEROX PARC
- University of Minnesota for 17 years in the Department of Chemical Engineering and Materials Science before coming here in 2005
- Currently holds positions in Physics, Chemical Engineering, and Chemistry/Biochemistry
Research Interests

- Predicting and understanding the structure and properties of materials using quantum mechanics!
- Functionalization of nano-materials (doped nanowires, multi-wall carbon nanotubes, semiconductor oxides)
- Simulated imaging of experimental probe microscopy techniques (AFM/STM)
- Development of high performance algorithms to solve the electronic structure problem
Research Group

Chemical engineering, materials science, condensed matter physics, applied math

Pseudopotential Algorithm for Real-Space Electronic Calculations

http://parsec.ices.utexas.edu
Electronic materials can be functionalized by adding controlled amounts of “impurities” (called dopants). At small length scales, this procedure is not well understood. We use new numerical techniques to address such issues.
Ex: ZnO Nanocrystals

Diameter:
- 9 Å
- 11.9 Å
- 13.6 Å
- 14.4 Å
Understanding the nanoscale means knowing where the atoms are. Few theoretical tools are available for this task.
Imaging H-bonds!

8-hydroxyquinoline

Zhang et al., Science 341, 611 (2013)

Hydrogen bonds??
Progress in computational advances (hardware) keeps growing at a phenomenal rate, but not software! Why? Can we discover new ways of writing software?
We apply theory and modeling techniques to do the following:

- Understand properties of electronic materials
- Predict properties for designing new materials (functionalization)
- Capitalize on two “mega” trends--bigger computers and the need for novel materials
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Genius is one percent inspiration and ninety-nine percent perspiration! - Thomas Edison

If Mr. Edison didn’t perspire so much he would get more accomplished...knowing that a little theory and calculation would have saved him ninety per cent of his labor. - Nikola Tesla