Prof. Jim Chelikowsky

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Department of Chemical Engineering
Institute of Computational Engineering and Sciences

Student Presentations, March 2015

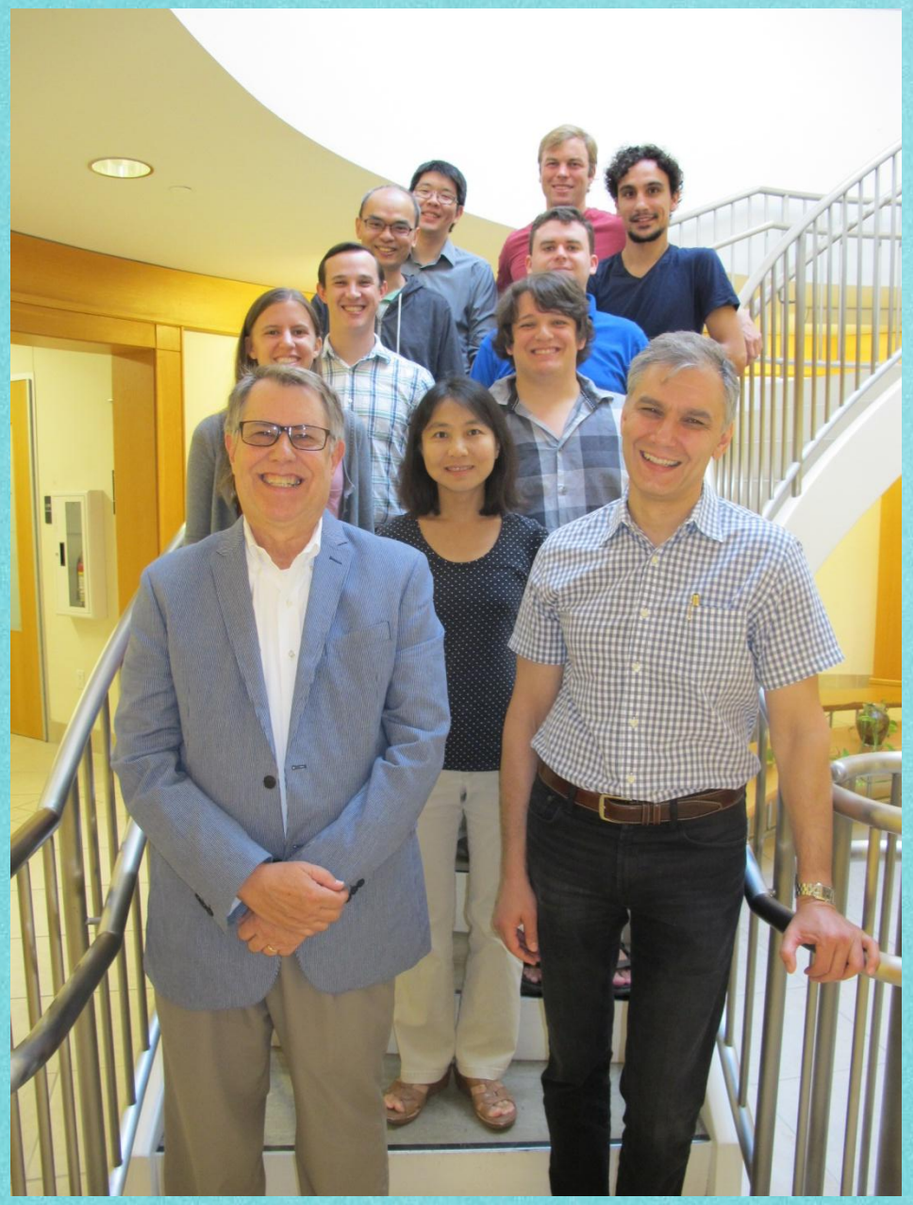
Academic and Professional Background

- **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**

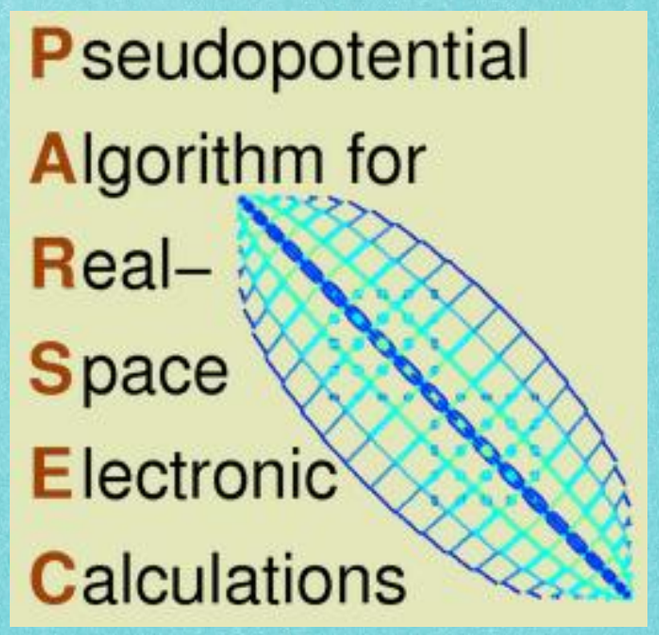
Research Interests

- ***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



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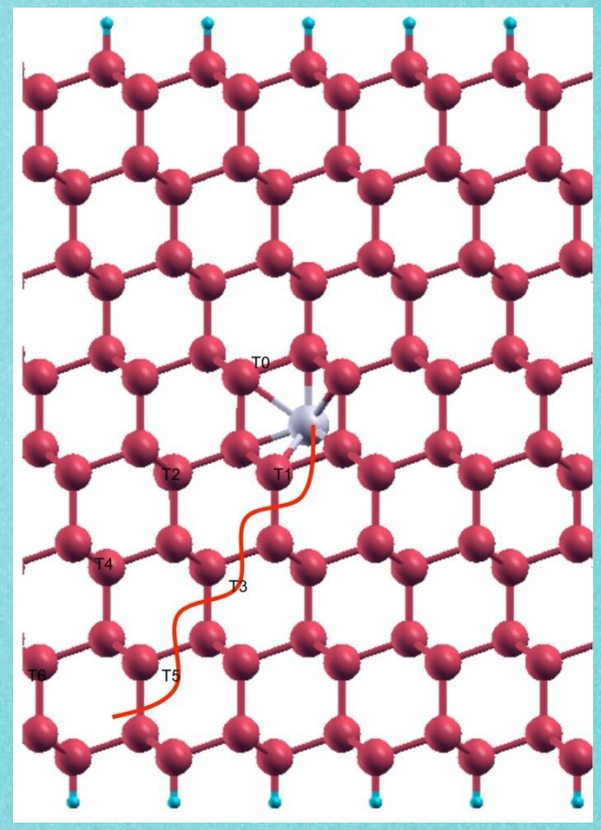
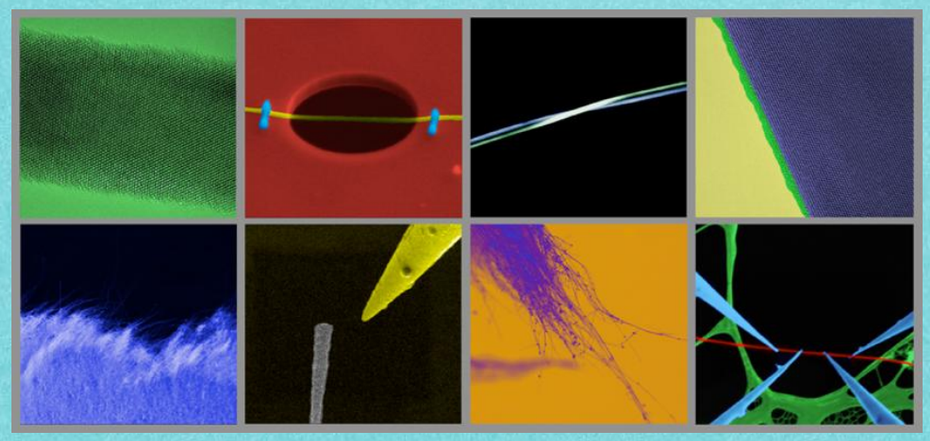
Functionalizing the Nanoworld

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.





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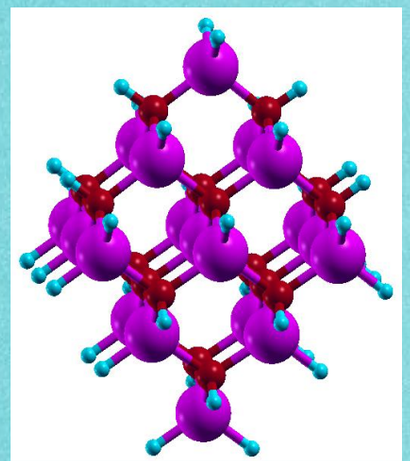
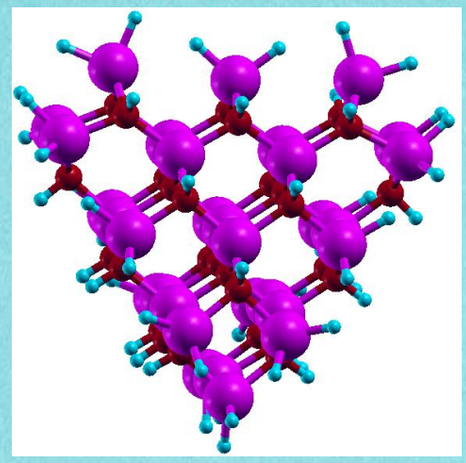
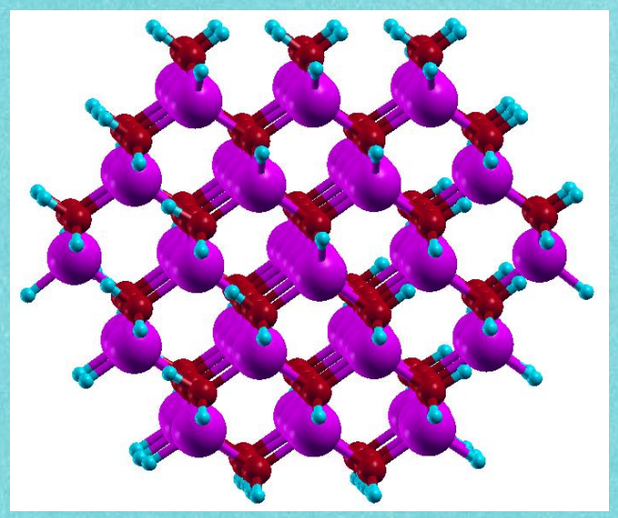
Ex: ZnO Nanocrystals



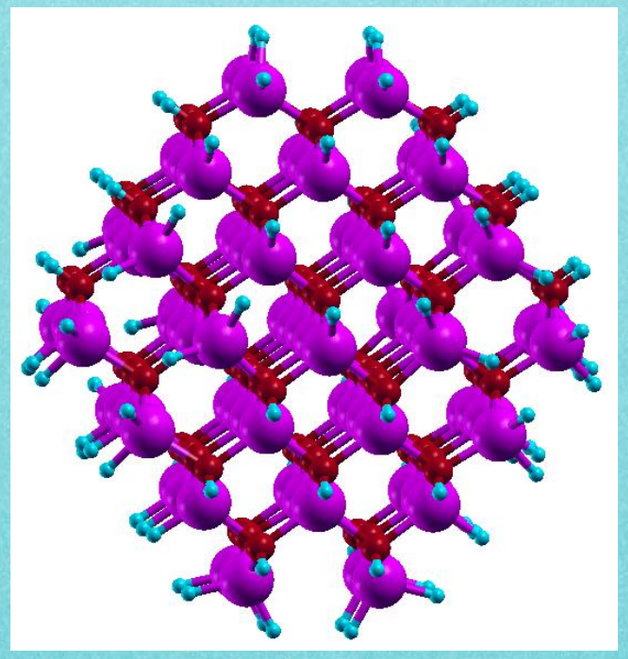
Dia. = 9 Å



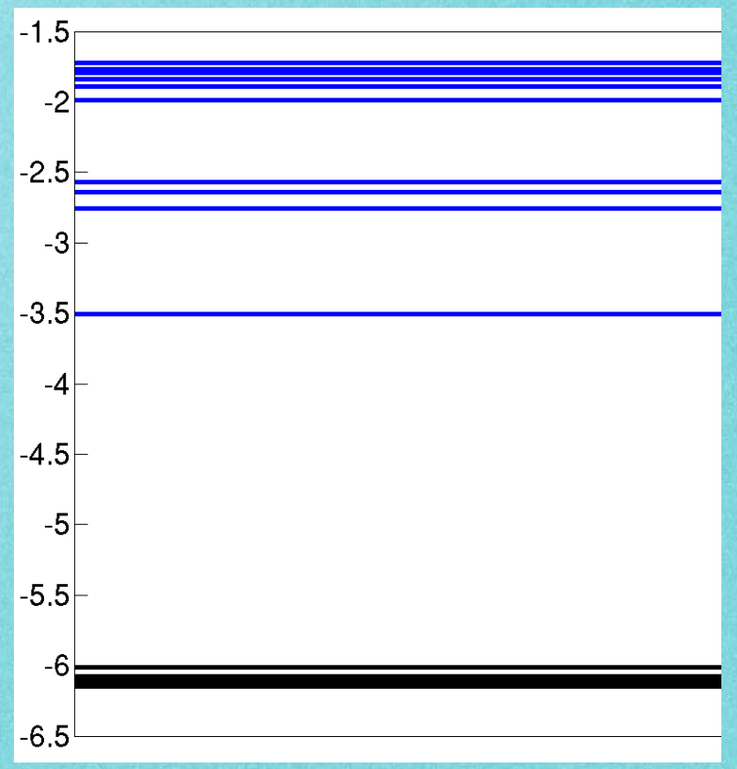
Dia. = 11.9 Å



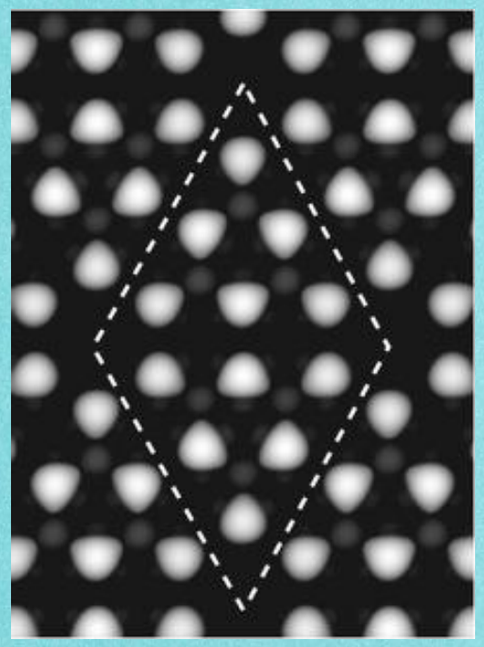
Dia. = 13.6 Å



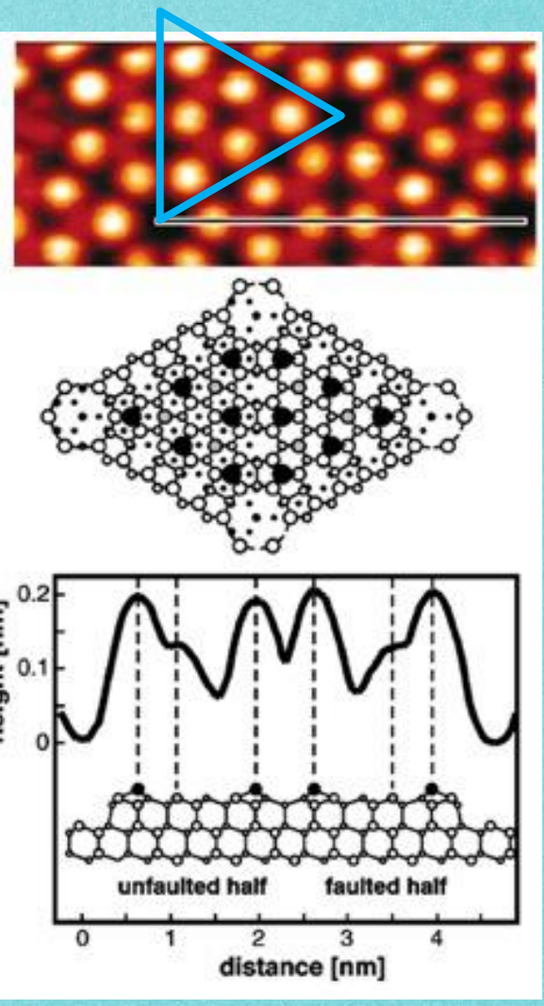
Dia. = 14.4 Å



Imaging the Atomistic World



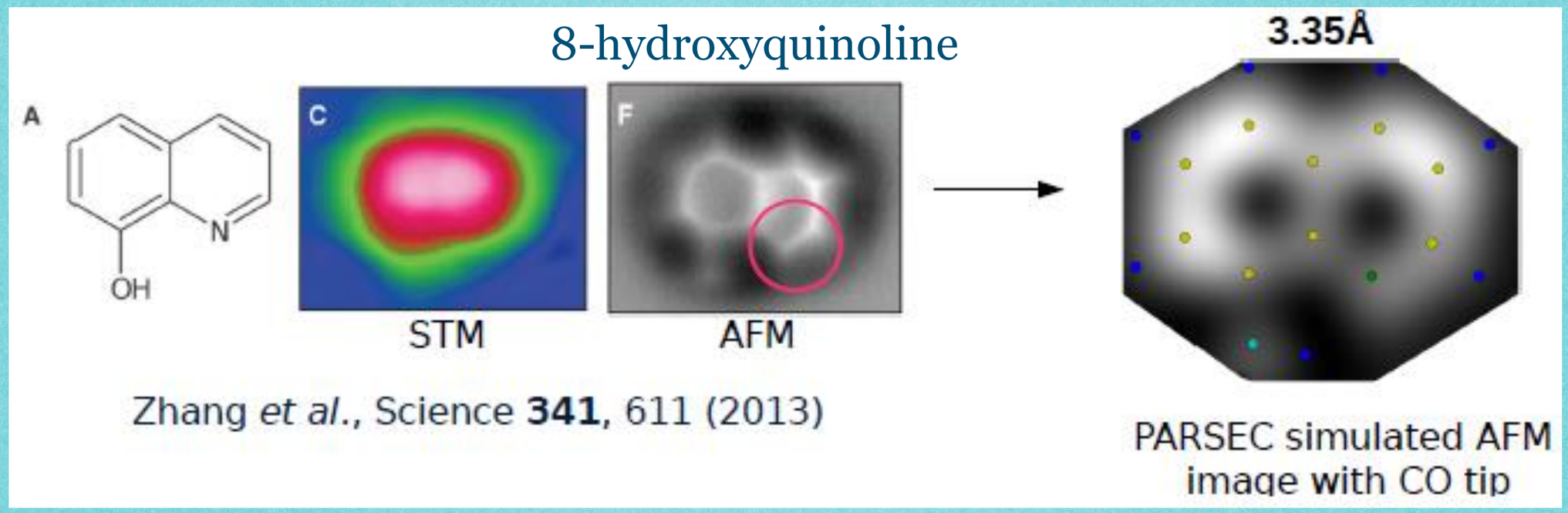
Theoretically simulated image of the silicon surface



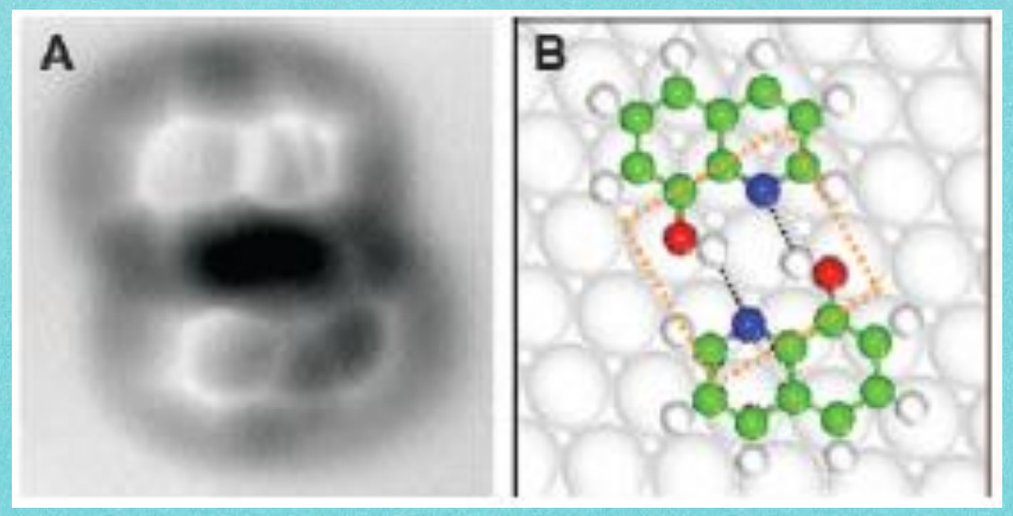
Experimental image of the silicon surface

Understanding the nanoscale means knowing where the atoms are. Few theoretical tools are available for this task.

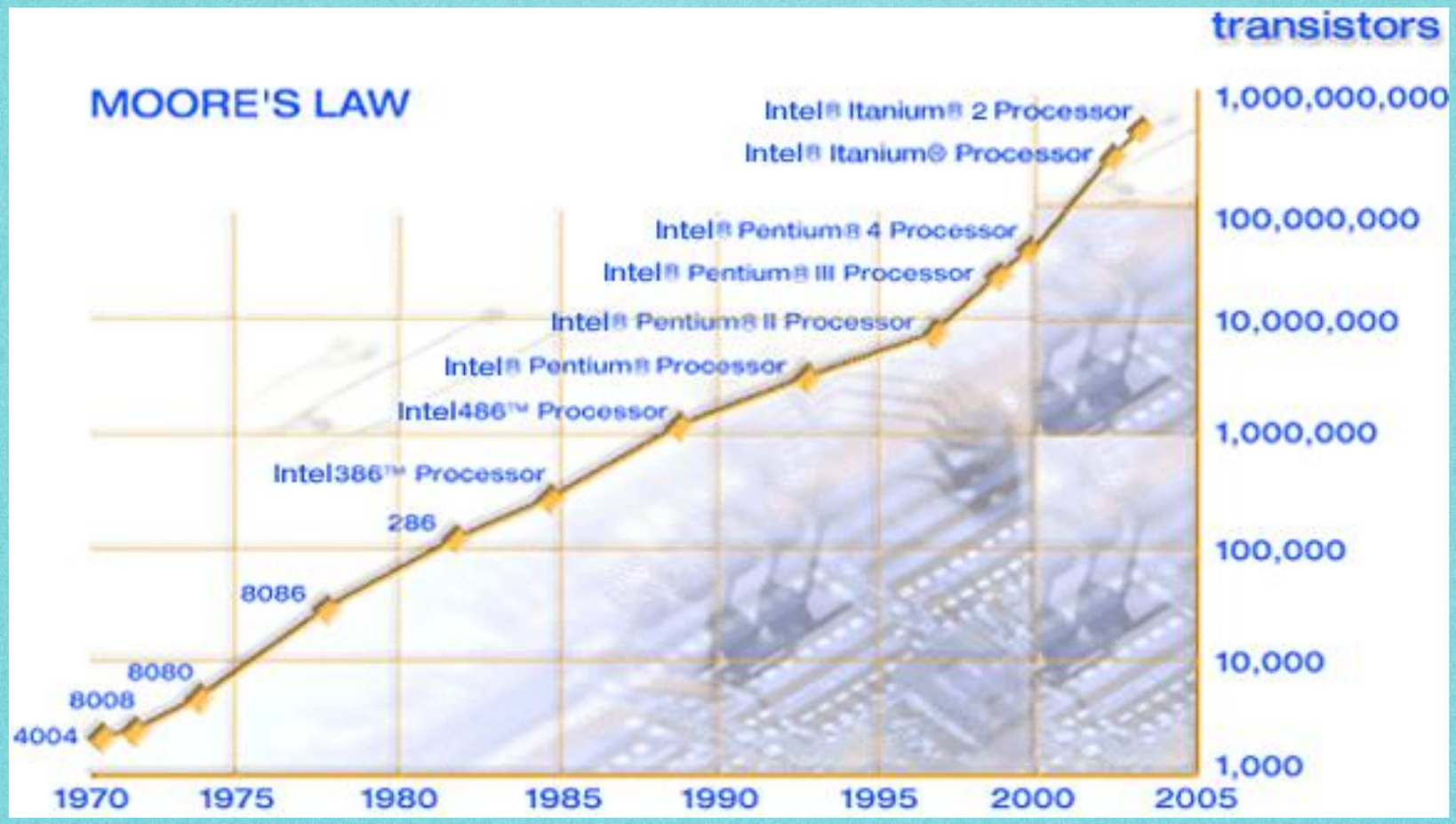
Imaging H-bonds!



Hydrogen bonds??



Software Development



Progress in computational advances (hardware) keeps growing at a phenomenal rate, but not software! Why? Can we discover new ways of writing software?

Summary!

- *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*

Contact

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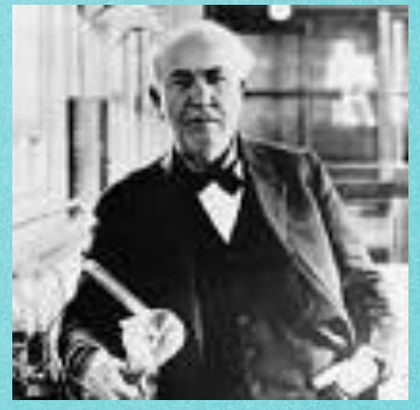
Genius is one percent inspiration and ninety-nine percent perspiration!- Thomas Edison



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