

# Prof. Jim Chelikowsky

Tex Moncrief Chair of Computational Materials



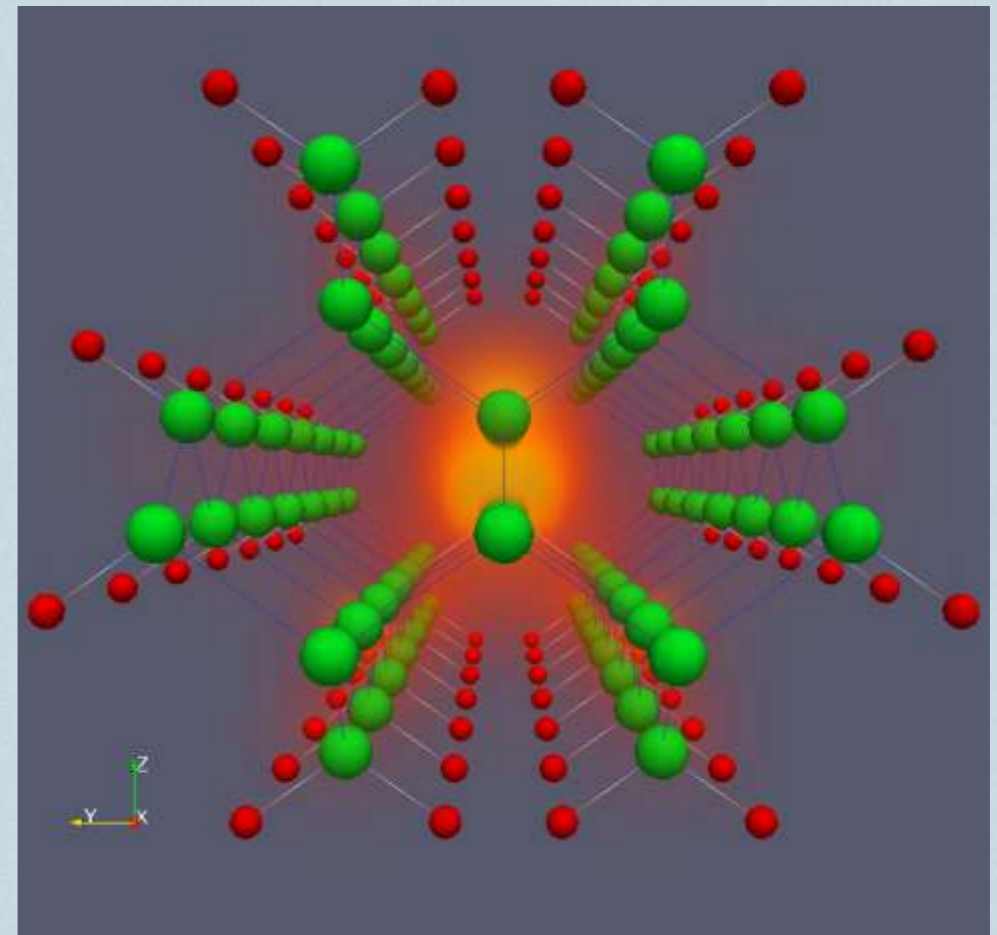
Department of Chemical Engineering, Center for Computational Materials within the Institute of Computational Engineering and Sciences



<http://tesla.ices.utexas.edu>

# Research Programs

- † **Software development for materials**
- † **Defects in oxide materials**
- † **Functionalization of nanostructures**
- † **Materials informatics**
- † **Liquids and crystal growth**





# Research Activities

- **Using computers we do the following:**
- **Understand properties of electronic materials**
- **Examine hypothetical or experimentally inaccessible regimes**
- **Predict properties and new materials**
- **Capitalize on two “mega” trends-- bigger computers and need for novel materials**

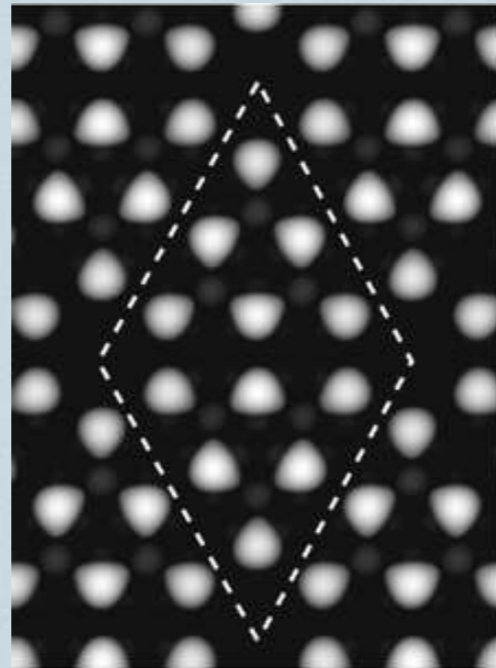


**Research group 2008:  
Multidiscipline**

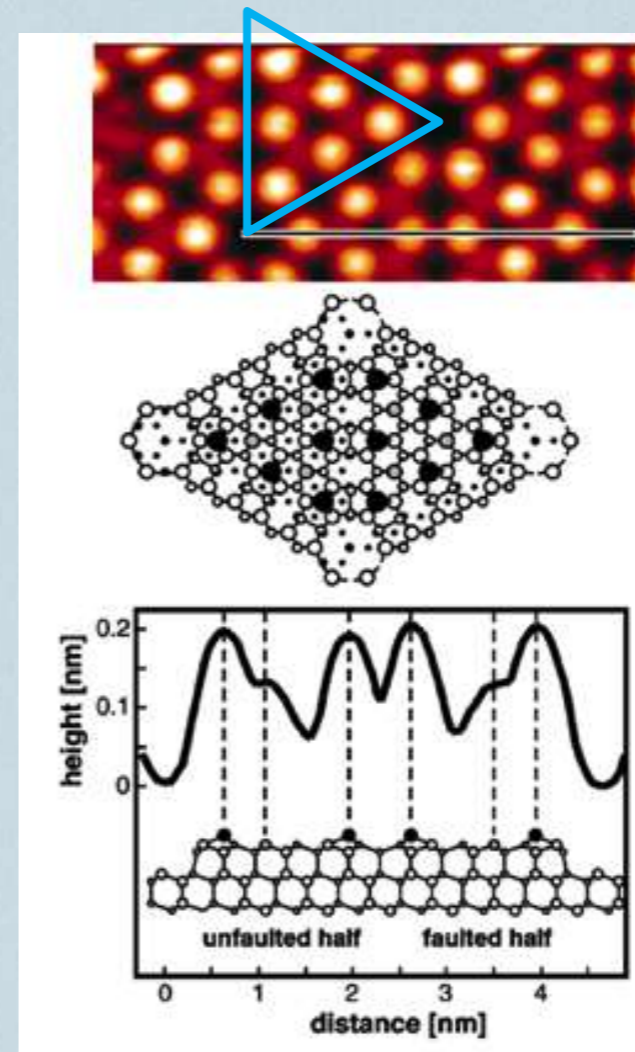
# Imaging the Atomistic World



Tzu-Liang Chan



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.