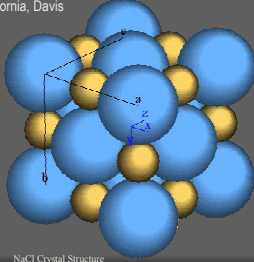


Experiment 1 – The Ionic Bond

ENG-45, Properties of Materials

Department of Chemical Engineering and Materials Science
University of California, Davis



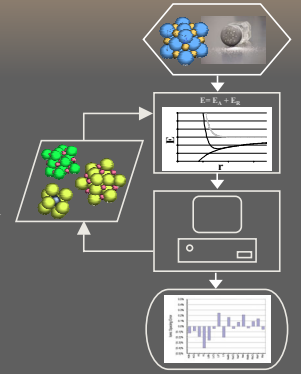
NaCl Crystal Structure

Man Camilleri and Mike Moser, 2004

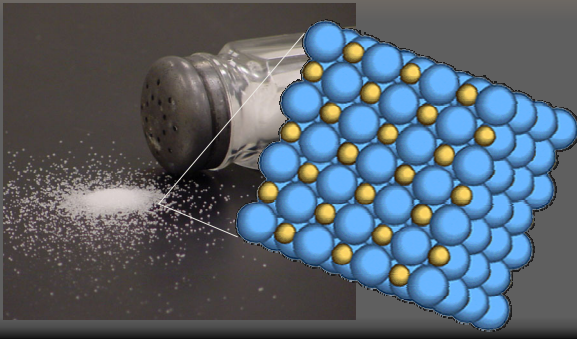
Objectives

Understand Bonding and Modeling:

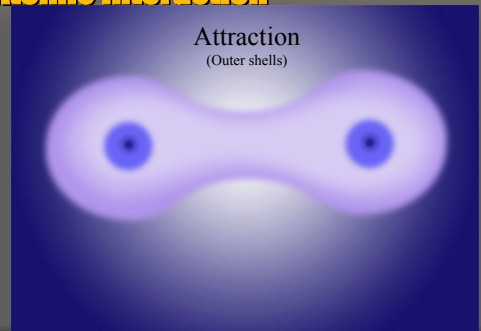
1. Atomic \leftrightarrow Macro
2. Spreadsheets modeling
3. Structured approach
4. Build, validate, and apply model



Atomic \leftrightarrow Macro

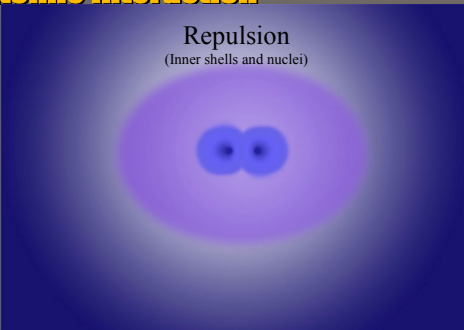


Atomic Interaction



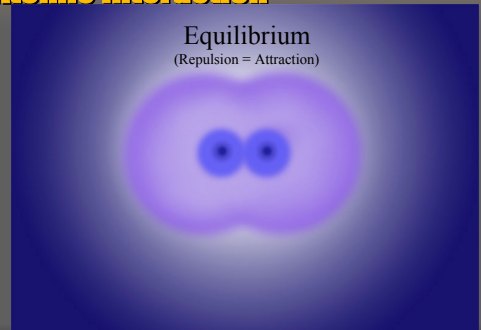
Atomic Interaction

Repulsion
(Inner shells and nuclei)

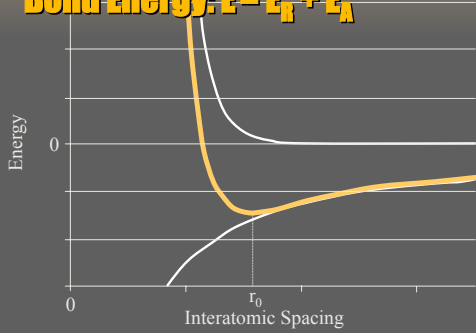


Atomic Interaction

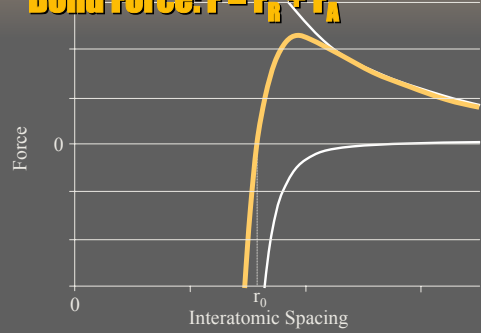
Equilibrium
(Repulsion = Attraction)



Bond Energy: $E = E_R + E_A$

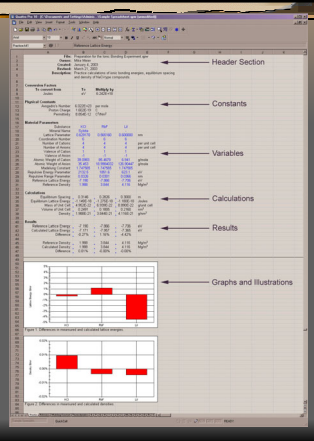
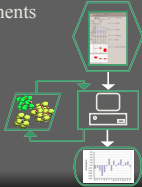


Bond Force: $F = F_R + F_A$



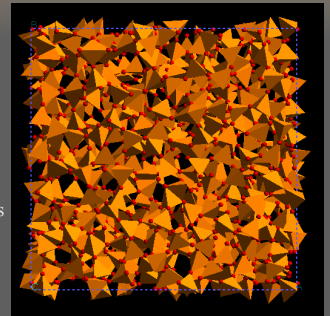
Modeling

- 1) Build spreadsheet model
- 2) Validate model
- 3) Use model for additional *NaCl*-type compounds
- 4) Compare to results from experiments



Summary

- Atomic → Macro
- Bonding → Properties
- Model vs. Experiment
- Applications
 - Manufactured molecules
 - Pharmaceuticals
 - Catalysts
 - Solid-state devices...



Random SiO₂ tetrahedrons; Image by Liliun Davila