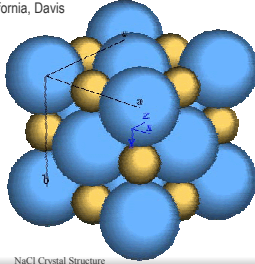


Experiment 1 – The Ionic Bond

ENG-45, Properties of Materials

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



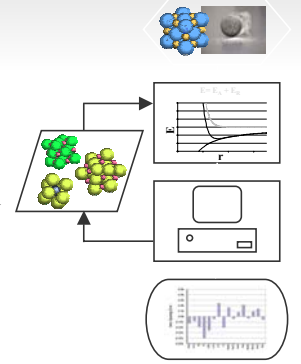
NaCl Crystal Structure

Matt Camilleri and Mike Meier, 2004

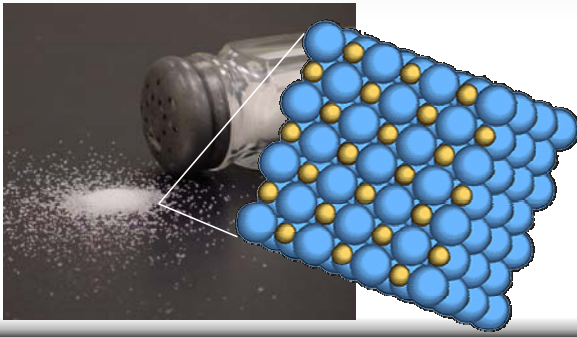
Objectives

Understand Bonding and Modeling:

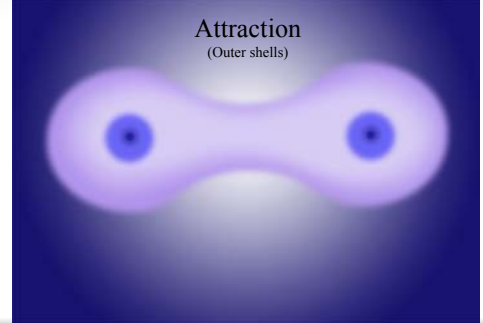
1. Atomic \leftrightarrow Macro
2. Spreadsheets modeling
3. Structured approach
4. Build, validate, and apply model



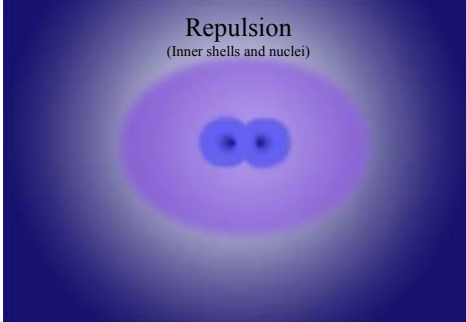
Atomic \leftrightarrow Macro



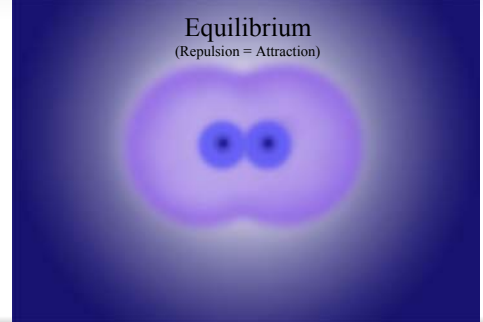
Atomic Interaction



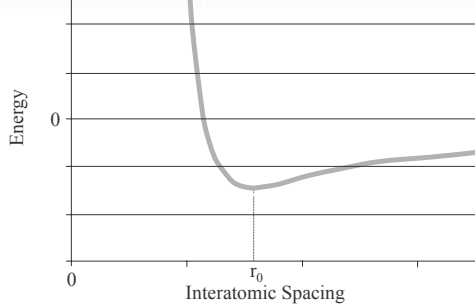
Atomic Interaction



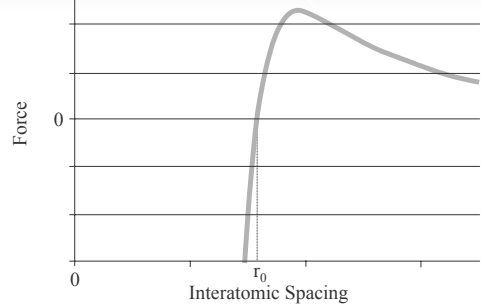
Atomic Interaction



Bond Energy: $E = E_R + E_A$

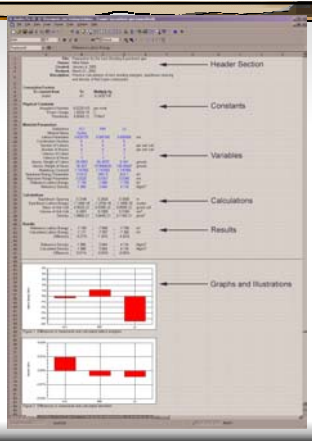


Bond Force: $F = F_R + F_A$



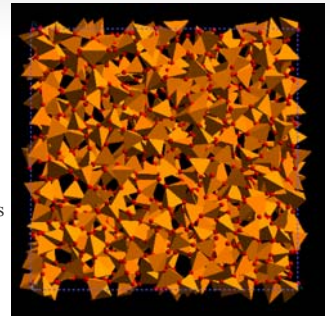
Modeling

- 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 Lilian Davila