Illustrating Molecular-Level Phenomena and Molecular Simulation Techniques with Commonly Used Software

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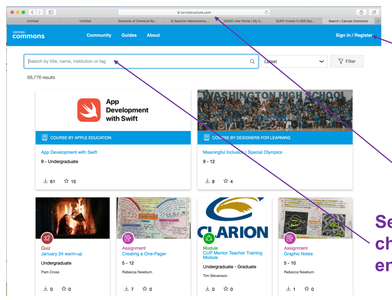
Motivation

- **Many grand challenges facing chemical engineers today involve molecular-level chemistry**
- **Having an appreciation for molecular-level phenomena will better prepare chemical engineers to handle problems in energy, water, food, catalysis, advanced materials, and other fields**
- **A major impediment to teaching and learning about molecular-level phenomena is the learning curve associated with molecular simulation software**
- **The goal of this work is to demonstrate molecular phenomena and simulation techniques using straightforward graphical user interfaces and familiar software**
- **Specifically, we focus on conceptual aspects of molecular-level chemical engineering, including students' abilities to connect molecular-level phenomena with observable properties**

All assignments (and more!) are available for public use on Canvas Commons. Search for "chemical engineering".



Materials are publicly available; no account necessary

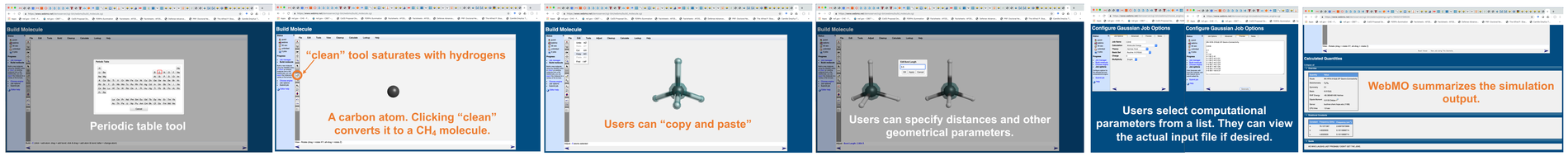
Navigate to lor.instructure.com

Search for chemical engineering

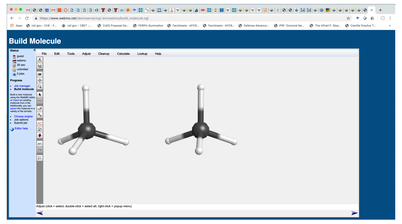
Example Assignment #1: WebMO/Quantum Chemical Calculations/Intermolecular Forces

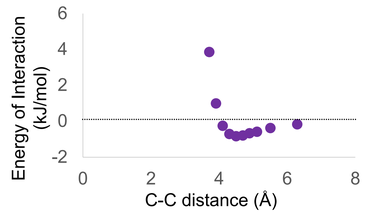
Objectives:
- Improve students' understanding about how pairs of molecules orient during intermolecular interactions
- Improve students' perceptions of quantum chemistry software
- Illustrate how intermolecular interactions are quantum in nature.
- Illustrate physical bonding and the use of the Lennard-Jones potential for modeling physical bonding.
- Determine correlations between physical bond strength, Lennard-Jones parameters, and physical properties

Students use WebMO, which uses an online graphical user interface, to set up and submit molecular simulations. WebMO was created by William F. Polik and Jordan R. Schmidt at Hope College. Anyone in the world can run WebMO with just an Internet connection.



Students place two CH_4 molecules in proximity and then "drag" them apart, calculating the energy of interaction at each point.



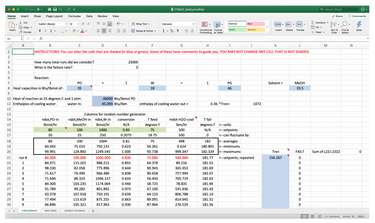


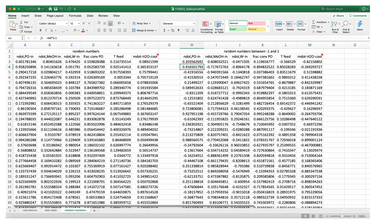
- Students complete a pre-assessment that re-enforces concepts from general chemistry, such as intermolecular forces and how they correlate to properties such as molecular weight
- After completing the pre-assessment, students work in pairs to calculate energies of interaction for pairs of molecules
- Each pair of students works on a different pair of molecules
  - Example molecule pairs: Ne-Ne, CH_4-CH_4, C_2H_6-C_2H_6, CCl_4-CCl_4, HCl-HCl, H_2O-H_2O, H_2S-H_2S, HCl-Ar, HCl-H_2O
- Before running the simulations, students sketch (by hand) what they think the optimal orientations of the molecules are
- Students also list the types of intermolecular forces that are present in the interaction
- While completing the assignment, students use the "pilot/navigator" approach to problem solving
- After completing the assignment, 2-3 pairs of students are combined into a bigger group to compare results.
  - Examples of larger groups: Ne-Ne, H_2S-H_2S, H_2O-H_2O; CH_4-CH_4, CCl_4-CCl_4, C_2H_6-C_2H_6; HCl-HCl, HCl-Ar, HCl-H_2O
- The larger groups are asked to write a paragraph describing the differences in the results in the context of the different intermolecular forces

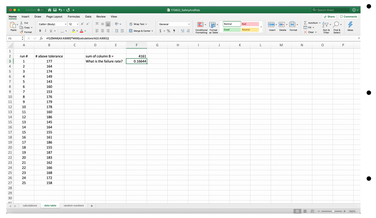
Example Assignment #2: Excel/Monte Carlo/Safety and Risk

Objectives:
- Illustrate how process variables influence process outcomes
- Introduce or re-enforce reaction runaway and chemical reactor safety
- Practice chemical engineering design, particularly the balance between safety and maximizing production rate
- Introduce the method of Monte Carlo using familiar software

Students use the random number generator and "data table" functions in Excel to calculate the temperature of a reactor for 25,000 different sets of conditions.





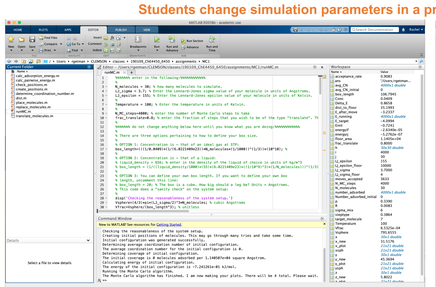


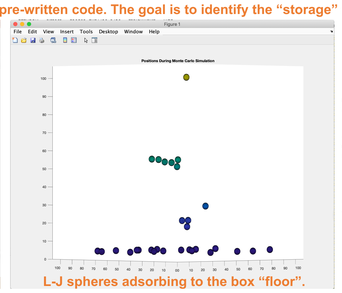
- Before completing the exercise, students complete a module that describes how Monte Carlo is used for various applications from sports to molecular adsorption
- During the exercise, students calculate the number of "failures" for a base case
  - Failure occurs when the reactor temperature exceeds a certain value
- Students then change different process variables until they achieve a failure rate of 0.

Example Assignment #3: MATLAB/Monte Carlo/Temperature Swing Adsorption

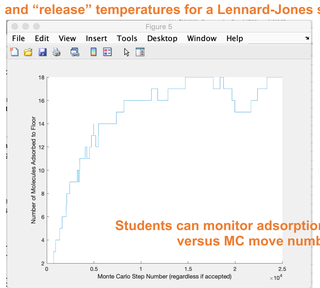
Objectives:
- Practice using Monte Carlo for molecular applications, including practicing operating the most important simulation parameters (intermolecular potential, temperature, number of moves, ratio of translate to replace moves)
- Demonstrate how the simulation parameters influence the number of moves required to achieve equilibrium
- Introduce the concepts of temperature swing adsorption and adsorptive separations. Learn how to tune operating conditions to achieve optimal performance for these two applications.
- Demonstrate how molecules with different interaction strengths exhibit different adsorptive properties.
- Develop an appreciation for how results obtained in a molecular simulation can be transposed to experimental or real world operation (e.g., trends rather than exact values)
- Improve students' perceptions of and confidence in installing and using MATLAB

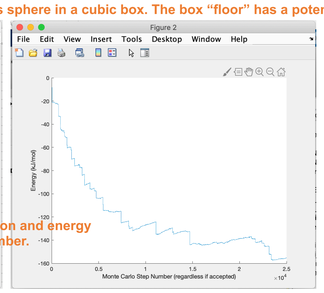
Students change simulation parameters in a pre-written code. The goal is to identify the "storage" and "release" temperatures for a Lennard-Jones sphere in a cubic box. The box "floor" has a potential representative of a sorbent material.



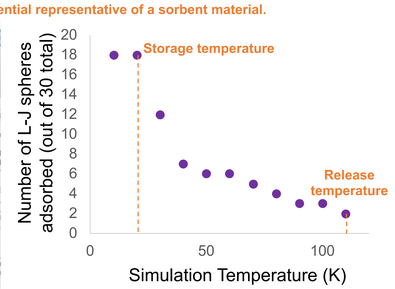


L-J spheres adsorbing to the box "floor".





Students can monitor adsorption and energy versus MC move number.



Other Available Assignments

- **Students use WebMO to find the transition state for HCN isomerization to CNH**
  - **Demonstrates transition state theory, transition state structures, reaction coordinates, use of quantum chemical calculations, vibrational modes**
- **Students use WebMO to calculate the energy levels of a 3d metal atom**
  - **Demonstrates quantized (versus continuous) energy levels, quantum chemical calculations, deciding how to choose basis sets and methods of electron correlation, solutions to the Schrödinger equation**
- **Students use WebMO to calculate electronic, vibrational, translational, rotational contributions to the energy, and free energy for H, O, and H_2O**
  - **Demonstrates statistical mechanics, different contributions to the energy and entropy as functions of temperature, quantum chemical calculations, deciding how to choose basis sets and methods of electron correlation**
- **Students use a Monte Carlo algorithm in MATLAB to predict the outcomes of the March Madness (basketball bracket)**
  - **Demonstrates configurational disorder, configurational entropy, ensembles, and intentional biasing ... AND promotes women's basketball!**

Coming soon: All MATLAB assignments will be converted to Python to promote Open Educational Resources

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