The Study $\pi$-Stacking Interactions
An Overview of Stacking

• What is $\pi$-Stacking?
• It is the interaction between aromatic rings
  • *It is non-Covalent*

• This is a simple example of a covalent interaction.
What are aromatic rings?

- They are simply rings that have a resonance structure.
π-Stacking can determine the conformation of Dimers

This example shows different conformations of a benzene dimer

Sandwich  T-shaped  Parallel-dispaced

What factors control these interactions?
Dr. Houk and Dr. Wheeler’s Research

- They replaced a benzene ring with a Hydrogen atom.

- The interaction energies were nearly identical.

- How were these energies calculated?
By solving Schrödinger’s equation.

\[
\left[ \frac{-\hbar^2}{2m} \nabla^2 + V \right] \Psi = i \hbar \frac{\partial}{\partial t} \Psi
\]

• Solving this by hand for the entire dimer would be near impossible.

• Schrödinger’s equation is solved numerically using a computer
About EOS

- It is a 3168 core cluster each core operates at 2.8GHz
  - 324 quad cores Nehalem Processors
  - 48 six core Westmere processors
- 372 nodes total
Current Research

- Creating Data
- Adding substituents
- See how the stacking interactions change.