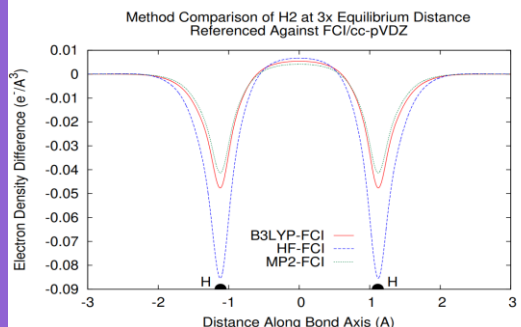
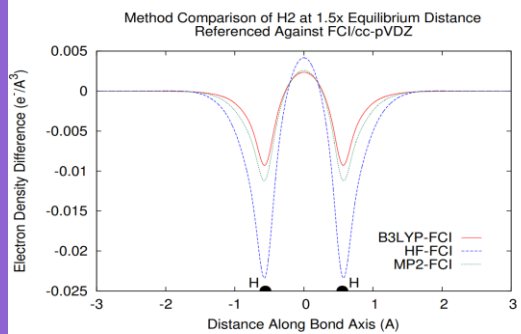
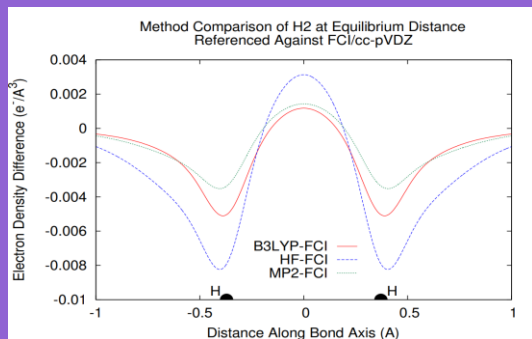
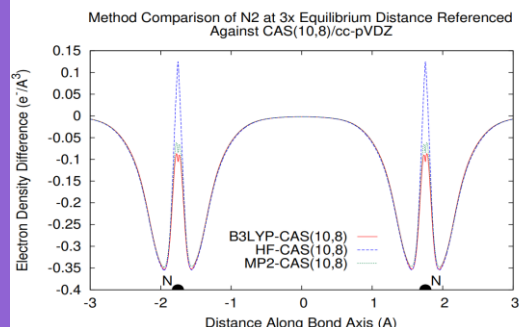
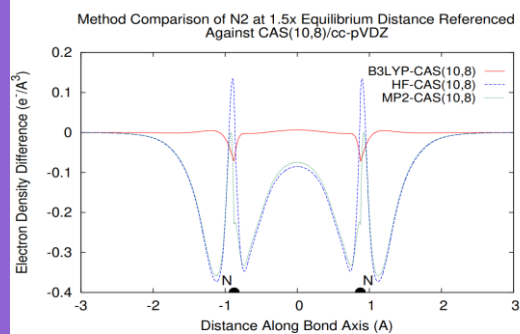
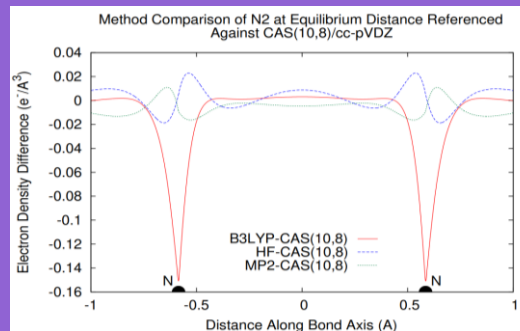


Comparing Computational Methods by Stretching Diatomic Molecules

Comparing the electron density profiles of H2 and N2 at various bond lengths

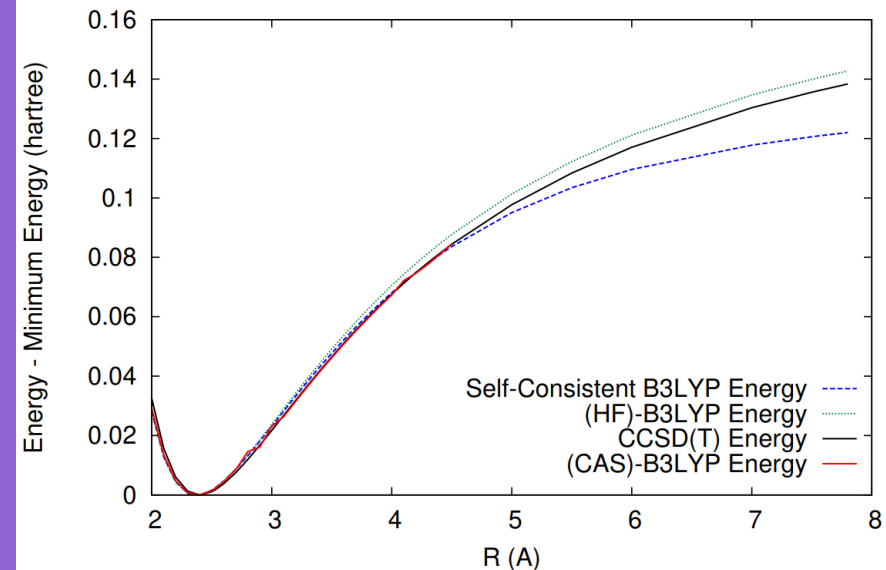


Increasing bond length



Comparing new (CAS)-B3LYP method with known methods from literature

Dissociation Curves of NaCl Using Various Computational Methods



- Goal was to improve upon recent literature technique (Green/dotted)
- Troubles converging calculations at $R > 4.5$ (Red)
- Results Inconclusive, more work to be done