

A Look into Titan

Using CPMD to simulate conditions
of Titan

Summer Project

My project was to use the software program CPMD to run simulations of atoms.

Goal of Project

The objective of the project is gain a better understanding of how atoms may interact on Titan in the presence of high energy and to see if complex molecules might be created on Titan.

Specifics of Project

240 atoms were used for the project. This is from 20 molecules of water, methane, and ammonia, which gives 20 atoms of oxygen, carbon, and nitrogen and 180 atoms of hydrogen.

The simulations are run at 50,000K. This is to break hydrogen-hydrogen bonds and run the simulations at high energy.

Facts of Titan

- The composition of the atmosphere is 95% nitrogen gas and 5% methane. There are other organic compounds in the atmosphere at very low rates.
- The temperature and pressure of the atmosphere is 95K and 1.5 bar.
- Titan has methane lakes across its surface.
- The interior of Titan is composed about half of water ice and silicates.
- Titan is the largest satellite of Saturn.

Methods- Density Functional Theory

All atoms are composed of a nucleus and electrons. Electrons are tiny, negatively charged particles. They are particles that also have wavelike properties.

The movement of electrons can be described by the wave function. With more than one electron, the functions that govern these electrons get more complicated due to the repelling nature between the particles. Density Functional Theory is a tool that maps out the electronic structure of the atoms. Ab initio is a process that calculates the wave function of the electrons.

Methods-CPMD

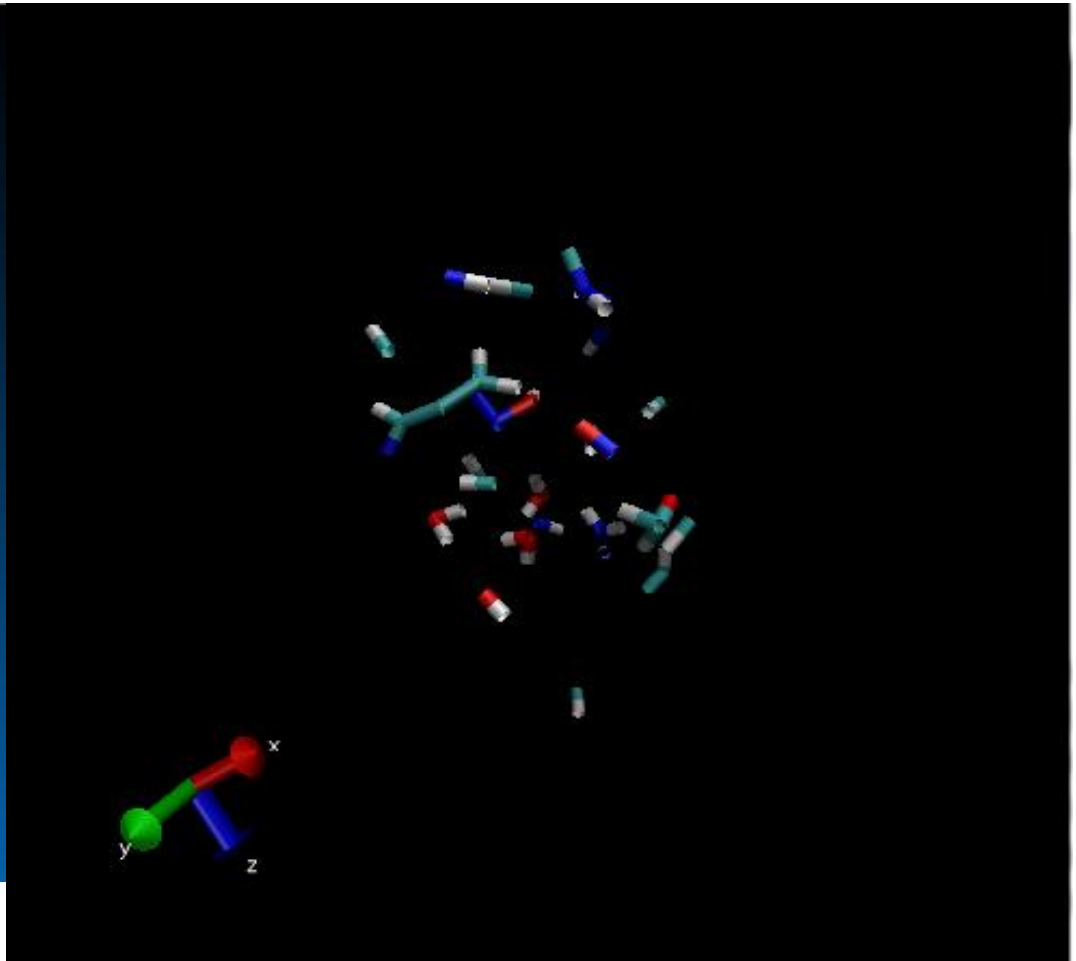
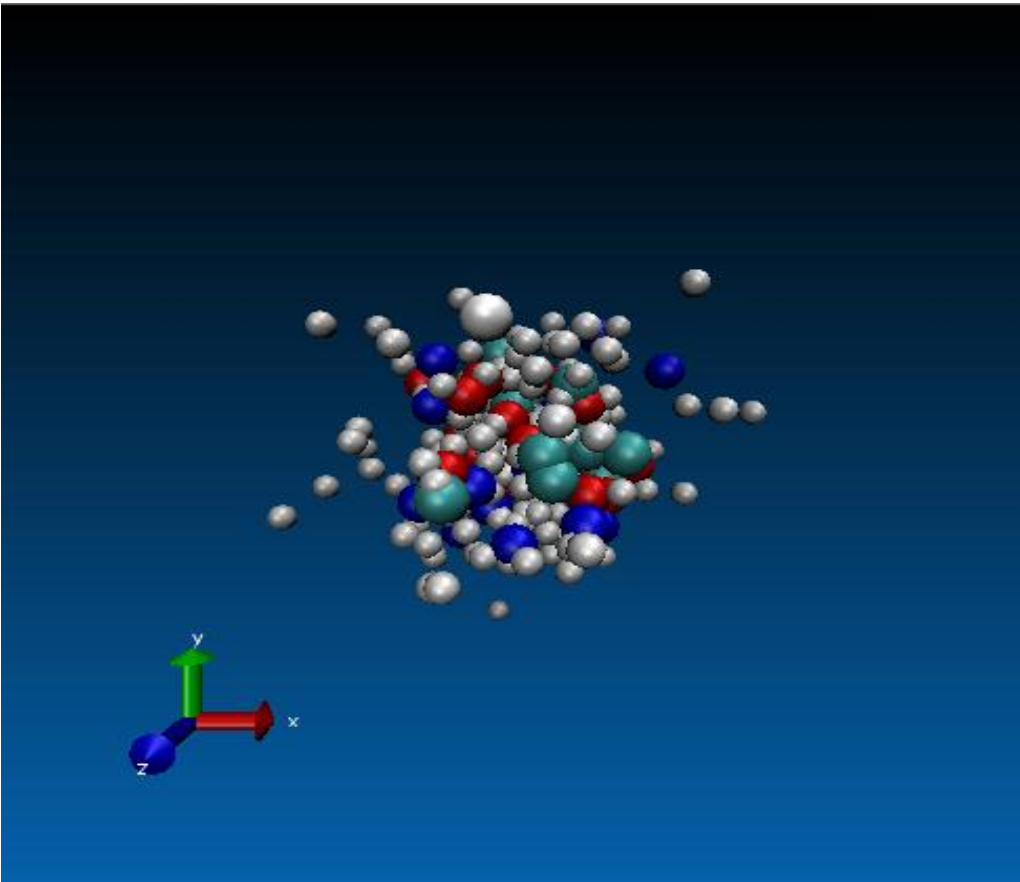
CPMD, Car-Parrinello Molecular Dynamics, is a software package that calculates ab initio molecular dynamics.

I used the software to optimize the geometry of the molecules, optimize the wave functions of the electrons, and run molecular dynamics of the molecules.

Results

The molecular dynamics will be looked at in two ways. One will be visually. The other way will be with respect to energy. For visuals, the atoms will be shown, and the bonds will also be shown.

Results



What I Have Learned

I have learned many new skills and ideas. I have learned how to operate Unix and its structure. I have learned many commands for it and feel very comfortable to use it. I have learned how to use CPMD and run simulations. I have learned how to write input files and scripts. I have learned some DFT. These were things that I had no knowledge of or proficiency with before I came.

Credit

I have been greatly helped this summer by my research adviser Dr. Pratt and by Dr. Hoffman.