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Friction of (110) Diamond in the Presence of Small Hydrocarbon Molecule

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SENIOR THESIS APPROVAL

This Honors thesis entitled

"Friction of (110) Diamond in the Presence of Small Hydrocarbon Molecule"

written by

Catherine Manning

And submitted in partial fulfillment of the
Requirements for completion of the
Carl Goodson Honors Program
Meets the criteria for acceptance
And has been approved by the undersigned readers.

Dr. Martin Perry –Thesis Director

Dr. Terry Sergeant – Second Reader

Mr. Glenn Good – Third Reader

Dr. Doug Reed – Honors Program Director

April 14, 2000

Friction of (110) Diamond in the Presence of Small Hydrocarbon Molecules

Catherine Manning

April 15, 2000

Contents

Abstract

Molecular dynamic simulations have been used to explore the friction between two (110) diamond surfaces in sliding contact. In general, when a third-body hydrocarbon molecule is placed between two computer generated diamond surfaces in sliding contact, the result is a reduction of friction as the load is increased compared to the same surfaces in the absence of third-body molecules. The size, shape, and alignment of the third-body hydrocarbon molecules play an essential role in the reduction of friction. Results for a system with ethane presented as a third-body molecule will be compared to previous theoretical studies as well as existing experimental data.

1 Introduction

Diamond is used because it has unique friction and wear properties. Diamond coatings are used throughout the industrial world, from drill bits to computer chips. With new information about how diamond surfaces break down, the industrial world could be changed forever; no longer would expensive drill bits need to be replaced or engine blocks melt due to heat. Another use for diamond related technology is the creation of synthetic diamonds. Synthetic diamonds could be used to protect the shuttle from space debris or to withstand the high temperatures of re-entry[1].

Tribochemistry is the interaction of chemistry and friction. Friction occurs when two bodies slide past each other. Sometimes when bodies slide past each other they produce debris. With the increase of debris, the coefficient of friction is increased. Science has made great strides in understanding tribochemistry at the atomic level. It has been observed in macroscopic experiments that when two diamond surfaces are sliding, they initially produce a small amount of friction, however, as the sliding continues, the friction increases resulting in the breaking of bonds[2]. It has been concluded that with the breaking of chemical bonds there is the creation of radical sites[2]. With the creation of radical sites on both surfaces, bonds are created between the two surfaces thus increasing the friction and eventually the temperature of the system. To fully understand what happens in this macro-experiment, the experiment was simulated with the help of a computer. With the computer, the position of any given atom in the system is easily determined at any specific point in time[2].

With new developments in scientific instrumentation and chemical vapor deposition, the growth of diamond films can now be understood at the microscopic level[3]. Thus, the advances in "wearless" diamond surfaces are just around the corner with the help of new scientific instruments like the surface force microscope[4] and the quartz crystal microbalance[4]. On the theoretical level of developments, molecular dynamics are being used to explain the wear and distortion of a diamond surface when sliding occurs. [5]

In previous experiments, the friction and wear of a diamond surface has been explored using molecular dynamics. The surface of diamond that has been the main subject of study is the (111) surface; therefore, the focus of this paper is the (110) surface[6]. With each additional diamond surface that is explored with or without the addition of a third-body molecule, the results bring us one step closer to developing a "wearless" surface. [4]

2 Methodology

2.1 Molecular Dynamics

Molecular dynamics simulations are used "to examine the friction between two surfaces placed in sliding contact.[5]" Molecular dynamic simulations are used to gain insight into what happens at the molecular level when atoms or molecules come in contact with each other.

2.2 Simulations

Molecular dynamic simulations were used in this study to examine the (110) hydrogen terminated diamond surface. Each surface is composed of exactly 176 carbon atoms and 16 hydrogen terminating atoms. The atoms in each diamond surface are divided into three regions: rigid, thermostat, and dynamic. The rigid layer is located at the other end from the hydrogen terminated carbons (the dynamic layer). The thermostat layer is located in between the dynamic and rigid layers (figure 1). The dynamic layer also includes the third-body molecule that is inserted between the two surfaces if a third-body molecule is present. The diagrams in the appendix show the two diamond surfaces and the third-body molecule. In the figures the black atoms are the carbon atoms of the diamond lattices. The white atoms are the hydrogen atoms that terminate the diamond surfaces. The third-body molecule is in between the two surfaces. The molecular formula for ethane is C_2H_6. The two carbon atoms of the ethane molecule are represented in blue, while the hydrogen atoms are represented in red. The rigid layer is held fixed, thus allowing no movement. With each additional simulation, the diamond lattices are moved closer together to increase the load, thus, increasing the friction. The thermostat layer allows for movement; however, the velocities are reset to allow heat to be dissipated from the system. The dynamic layer allows for free movement. With the integration of Newton's equations of motion, the forces can be determined in each direction (F_x,F_y,F_z). Using this data the graphs can be generated that will show the normal and frictional forces for each simulation. The rigid layer is the layer that is moved in a simulation; however, the atoms remain at a constant relative distance. The way in which a simulation is performed is by holding one diamond surface in place and sliding the other in a given direction subject to periodic boundary conditions. Each simulation reveals the force generated in each direction and the friction coefficient that was measured as sliding occurred.

2.3 Potential Energy Function

The model was developed by determining an empirical potential energy function that explains the chemical bonding of hydrocarbons. The function must reproduce the intra-molecular energetics and bonding, "yield realistic energetics and bonding for structures, and allow for bond breaking and formation."

2.4 Tersoff Bond-order Expression

The Tersoff bond-order expression was used in the current molecular dynamic simulation. The Abell-Tersoff[7] formula is:

$$E_b = \frac{1}{2}\sum_i E_i$$

contribution of E is written as:

$$E_i = \sum_{j \neq i}[V_R(r_{ij} - B_{ij} * V_A(r_{ij})]$$

j and i are neighbors.
$V_R(r)4$ and $V_A(r)$ are paired repulsion and attractive interactions.
B_{ij} is a many-body coupling between atoms i and j.
The first approximation of B_{ij} is:

$$B_{ij} \alpha Z^{-\sigma}$$

σ is dependent on the system.

This gives the relationship between bond length, binding energy and coordination for systems containing carbon-carbon bonds.

The major problem with this expression is that the expression does not take into account the intermediate bonding situations. The Abell-Tersoff expression assumes the "near-neighbor interactions combined with the sum over atomic sites results in non-physical behavior[7]." Another problem is non-physical behavior when double bonds are explored-both conjugated and non-conjugated. These problems can be solved through a new equation which results in the binding energies for hydrocarbons.

$$E_b = \sum_i \sum_{j(>i)} [V_R(rij - B_{ij} * V_A(r_{ij})]$$

where

$$B_{ij} = \frac{B_{ij} + B_{ij}}{2}$$

The repulsive and attractive terms are:

$$V_R(r_{ij}) = \frac{F_{ij}(r_{ij})De_{ij}}{(S_{ij} - 1)e^{\sqrt{2S_{ij}}} B_{ij}(r - Re_{ij})}$$

$$V_A(r_{ij}) = \frac{F_{ij}(r_{ij})De_{ij}}{(S_{ij} - 1)e^{\sqrt{\frac{2}{S_{ij}}}} B_{ij}(r - Re_{ij})}$$

$$f_{ij}(r) = \int_0^1 \frac{1 + cos(\frac{\pi(r - R1ij)}{R2_{ij} - R1_{ij}})}{2}$$

$$R1_{ij} < r < R2_{ij}$$

The results of the final equation were close to observed experimental values for hydrocarbons meaning that results generated from the computer simulations are very close to the experimental value [7].

3 Results and Discussion

3.1 Previous Results

When comparing results of the insertion of third-body molecules between diamond surfaces, the results are almost always the same. Hydrogen atoms from the surfaces bond, thus, producing hydrogen gas. Another option is the third-body molecule breaking apart and then binding to the diamond surface thus creating more friction. In the case of placement of two ethyl groups on one of the surfaces, the result was the formation of hydrogen gas and molecular debris[8]. Another phenomenon that was observed was the shearing of hydrogen atoms attached to the surface. After methane,

ethane, methyl radicals, ethyl radicals, and isobutane molecules were placed between the two diamond surfaces, it was concluded that the presence of a third-body molecule reduces the average frictional force compared with that of just two diamond surfaces[8]. This is a result of less interaction between the hydrogens of opposing surfaces. In a system with no third-body molecules, the hydrogens have large interactions that cause the carbon atoms of subsequent layers to be affected. If a third-body molecule is inserted, the interaction of hydrogen molecules is reduced[8].

3.2 Results

Molecular dynamic simulations have been used to explore the friction produced when two (110) diamond surfaces slide past each other. These simulations have been performed at 300 K and at a sliding speed of $1.0\AA/\mathrm{ps}$. The results vary based on the distance the surfaces are from one another.

In figure 2, the friction coefficients are plotted as a function of average normal load per rigid-layer atom for two systems. The two systems are a (110) diamond system with hydrogen-terminated carbons and a (110) diamond system with ethane inserted between the two diamond lattices. The data shows that with the addition of ethane the coefficient of friction is smaller as the load increases compared with that of the hydrogen terminated system. Thus, the addition of a third-body molecule helps to reduce the coefficient of friction in the (110) diamond system.

When exploring the force versus the sliding distance per unit cell, the interaction of molecules can be understood. The normal force, F_z, and the frictional force, F_y, are shown in figure 3. The maxima are the result of the increase of the repulsive interactions of the hydrogen atoms of the two diamond lattices. This result is due to the fact that the hydrogen atoms of the two surfaces have passed by each other. Thus, the minima are the result of the decrease of the repulsive interactions of the hydrogen atoms. This decrease of repulsive forces is a result of the hydrogen atoms being perpendicular to the other hydrogen terminated surface. With the increase of the normal load, the mechanical excitation also increases. If the mechanical excitation increases, so does the friction coefficient[4].

Figure 3 is very similar to the graph (figure 6) of simulation B. The graph (figure 3) shows the ethane molecule moving freely between the two diamond surfaces. The two diamond surfaces at this point are too far apart to cause any significant hydrogen-hydrogen repulsive forces. At this point there is no significant difference between the friction produced in a system with a third-body molecule and one without.

Figure 7 as compared with figure 4 shows the surface of the two diamond lattices coming closer together. The friction force does not show any great changes between the two simulations (figures 3 and 6). The frictional force is around 0-0.02 throughout the whole simulation. In figure 7 it is easy to see how the frictional force is increased by the contact interaction of the ethane molecule and the hydrogen surface of the diamond lattice. Figure 8 shows the ethane molecule floating between the surface. There is a great distance between the two diamond lattices, thus, there are few hydrogen-hydrogen repulsive forces.

In simulation C (figure 9) the frictional force has increased as compared with that of simulation B (figure 6). The surfaces of the diamond are even closer than they were before. The hydrogen-hydrogen repulsive forces are starting to play a bigger role in the overall frictional force that is being produced. In figure 10, the hydrogens of the ethane molecule are starting to get closer to the diamond surfaces. If compared with figure 11 the ethane molecule is interacting less with hydrogen atoms on the lattices as before. The ethane molecule throughout this entire simulation is still moving very freely as compared with that of higher load simulations.

Figure 12 looks very similar to that of figure 6. The overall frictional force is not increasing greatly through the previous trials. It appears that the surfaces of the diamond are not close enough to make a great deal of difference in the results. The high frictional force figure 14 shows a few hydrogen-hydrogen repulsive interactions. The low frictional force shows a very similar result to figure 11. The third-body molecule at this particular time in the simulation process is not playing a large role in the decrease of friction like it will later in the process.

The variation of the frictional force becomes apparent in simulation E (figure 15). It appears that the ethane molecule is starting to get stuck periodically when the two diamond lattice slide past one another. The surfaces are now close enough to have some hydrogen-hydrogen repulsive forces. Figure 16 shows the ethane molecule interaction with the hydrogen termination of the diamond surfaces. In figure 17, the ethane molecule appears to have a few interactions. Even though the ethane molecule is starting to have a greater role in the overall frictional force generated at two diamond surfaces, this simulation does not distort the ethane molecule so it is still considered a low load simulation.

In simulation F, there is still no distortion of the ethane molecule. The graph (figure 18) is starting to show a greater fluctuation in values as compared with that of figure 15. One could conclude that the surfaces are causing the ethane molecule to get trapped more often and with a greater time period when it is trapped. In figure 19, the ethane molecule is experiencing increased interactions with the hydrogen-terminated diamond surfaces. Immediately after the interactions, the ethane molecule slips into a valley; thus, resulting in a decrease in the overall frictional force of the system.

The graph (figure 21) in simulation G shows a significant oscillation at the beginning of the simulation. When the ethane molecule is in the valley, the friction coefficient is significantly lower. If the molecule interacts with the hydrogens on the surface of the diamond, then the friction is increased because of the hydrogen-hydrogen repulsive interactions.

In figure 24, the graph shows the force per sliding distance of a low load system. At its maxima the ethane molecule shows almost no deformation as compared with that of figure 43. The molecule appears to move without too many molecular interactions from the hydrogen terminated diamond surface in both figure 25 and 26. With the great distances between the surfaces there is relatively little hydrogen-hydrogen repulsive forces acting between the surfaces.

In figure 28, the ethane molecule experiences a great amount of deformation as compared with that of figure 25 or 26. The surfaces of the diamond lattices are closer together, thus affecting the ethane molecule and the hydrogen-hydrogen repulsive forces. In figure 29 one of the two carbon atoms of the ethane molecule has had its hydrogen atoms distorted.

Figure 30 shows a sharp increase in the normal force followed immediately by a minima. This is caused by the ethane molecule getting caught when the two diamond surfaces slide past each other (figure 31). The ethane molecule has fallen into a valley between the hydrogen terminated diamond surfaces (figure 32). This results in the reduction of interaction as shown in figure 30.

According to figure 35 the ethane molecule continues to be moved from a valley to being trapped on hydrogen atoms. Figure 34 shows the molecule trapped on a neighboring carbon atom. Figure 33 shows a great deal of oscillation of the normal force and the frictional force.

In figure 36, the graph shows that the molecule from the beginning gets stuck in a valley (figure 38), then only a few unit cells later it is causing a great deal of hydrogen-hydrogen repulsion as show in figure 37. The large peak is the result of the ethane molecule changing its orientation between the two diamond lattices. There is still no significant deformation of the ethane molecule as compared to later simulations.

In figure 41, the surfaces of the diamonds are closer together; thus, the ethane molecule will be less likely to be swept along as the surfaces slide past each other. The ethane molecule oscillates (figure 39) greatly in this simulation as compared with simulation L (figure 36). At the minima, around four unit cells, the ethane molecule is right in the middle of the two surfaces. At the point of greatest repulsive forces the ethane molecule is distorted (figure 40) and right in the middle of hydrogen-hydrogen repulsive force interactions. This simulation marks the beginning of the high load simulations due to the great distortion of the ethane molecule.

Figure 42 shows even greater evidence of the high load and distortion of the ethane molecule. A great repulsion forces the ethane molecule is distorted causes it to be planar (figure 43). There is great strain on the bonds of the ethane molecule (figure 43); yet, if the molecule is in a valley, the bonds return to their equilibrium position (figure 44). The greater the strain on the bonds the more likely the ethane molecule is to break apart.

In this simulation the maximas and minimas are more gradual. It appears to show the molecule moving and then staying in the location between the surfaces for a longer period of time. The ethane molecule appears to be moving more perpendicular to the surface of the diamonds (figure 46) under the high frictional forces.

With the increase in the load, the forces are changing even more drastically now. However, the amplitude between the changes is more constant now. At high frictional forces, the ethane molecule is perpendicular to the two diamond surfaces causing even more hydrogen-hydrogen repulsive interactions (figure 49). At lower frictional forces the molecule is deformed but in a valley on the surfaces; this results in less molecular interactions. Also, after the ethane molecule goes through the high frictional forces one of the hydrogen atoms from the surface of the diamond replaces one of the hydrogen atoms on the ethane molecule.

Figure 51 looks normal just like all the other trials but it is not. The ethane molecule dissociates in this simulation. The ethane molecule's carbon-carbon bonds break and the methyl radicals binds to the surfaces (figure 53). When the molecule binds to the diamond surfaces, the friction is greatly reduced. The friction is increased, however, when the two ethane carbons plus hydrogens termination come in contact with each other.

Simulation R does not fit the pattern of any of the other trials. When the molecule undergoes bond dissociation, (figure 56) the friction coefficient stays the same until the very end when it decreases again. It is almost as though the molecule binds to the diamond surfaces and then causes the surfaces to have even greater repulsive interactions. The friction is significantly higher in this simulation. At the minima the ethane molecule is in tact (figure 55). When the methyl radicals bind to the two diamond lattices, the radicals never recombine to form an ethane molecule. It bonds to the surfaces for the remainder of the simulation.

The results generated from this work closely resemble the results generated on other diamond surfaces[2]. It can easily be concluded that with the addition of a third-body molecule to a system the friction coefficient will be reduced when compared to a system without the molecule. The discovery of the changes of friction at the molecular level will help to further understand how to create "wearless" surfaces.

4 Conclusions

Molecular dynamic simulations were employed to study the friction produced at the atomic level of a (110) diamond surfaces. The two surfaces were in sliding contact and thermostatted at 300K. The results that were collected were compared with those of other diamond surfaces. It was found that the addition of a third-body molecule does in fact reduce the friction of the overall system as compared with that of a non-third-body molecule system. These results are consistent to those of other diamond surfaces that have been studied[4].

It was hypothesized that the addition of a third-body molecule would lower the total frictional force produced in the system. This was in fact the case. With the decrease in the distance between the surfaces, the third-body molecule was distorted from its original shape leading ultimately to the bond dissociation in the molecule. When this occurred the friction decreased for a short period of time. Later in the simulation, the third-body molecule's resulting radicals bonded to the surface of the diamond. It was concluded that the magnitude of the mechanical excitation depends on the molecule's shape and orientation during sliding. Another interesting conclusion that can be drawn is that when a third-body molecule is stuck in a "valley" on the surface of the diamond, the coefficient of friction reduces.

References

[1] Ivan Writer. Nanotechnology. *National Science and Technology Council*, pages 1–8, 2000.

[2] Judith A. Harrison and Donald W. Brenner. Simulated tribochemistry: An atomic-scale view of the wear of diamond. *Journal of the American Chemical Society*, 116:10399–10402, 1994.

[3] Martin D. Perry and Judith A. Harrison. Molecular dynamic studies of the frictional properties of hydrocarbon materials. *Langmuir*, 12:4552–4556, 1995.

[4] Martin D. Perry and Judith A. Harrison. Universal aspects of the atomic-scale friction of diamond surfaces. *Journal of Physical Chemistry*, 99:9960–9965, 1995.

[5] Martin D. Perry and Judith A. Harrison. The effects of methane-debris molecules on the frictional properties of diamond. *Science Publishers*, 1:109–119, 1995.

[6] J.A. Harrison C.T. White and D.W. Brenner. Effects of chemically-bound flexible hydrocarbon species on the frictional properties of diamond surfaces. *Journal of the Americal Chemical Society*, 97:6574–6576, 1993.

[7] Donald W. Brenner. Emprirical potential for hydrocarbons for use in simulating the chemical vapor deposition of diamond films. *Physical Review B*, 1:1–29.

[8] Judith A. Harrison and Martin D. Perry. The tribology of hydrocarbon surfaces investigated using molecular dynamics. *Kluwer Academic Publishers*, pages 1–15, 1997.

```
//***************************************************************************
//Author:  Catherine Manning
//Description:  This program takes a data file and changes the atoms into
//the correct color.  Hydrogen atoms are blue and carbon are red.
//***************************************************************************


//Libraries
#include<stdio.h>
#include<string.h>

//***************************************************************************
//Main program
//***************************************************************************
int main (){

  char line[100],blank[4];          //Line is the number in xyz direction
  int k,i,j;                        //Counters
  int frames=0;                     //number of frames
  int atoms=0;                      //number of total atoms
  int type=0;                       //hydrogen or carbon
  char x[25];                       //number in x direction
  char y[25];                       //number in y direction
  char z[25];                       //number in z direction

//***************************************************************************


  scanf ("%d",&frames);            //determines for number of frames
  scanf ("%d",&atoms);             //determines for number of atoms

  printf("%d \n", frames);         //print number of frames
  printf("%d \n", atoms);          //print number of atoms
  i=1;
  j=1;
  k=1;
  while (i<=frames){               //loop that prints first surface
     j=1;
     while (j<=192){
        scanf("%s ",&x);
        scanf("%s ",&y);
        scanf("%s ",&z);
        scanf("%d",&type);
        printf ("%s     %s     %s     %d\n", x,y,z,type);
        j++;
     }
    k=1;
     while (k<=8){               //colors the third body molecule
        scanf("%s ",&x);
        scanf("%s ",&y);
        scanf("%s ",&z);
        scanf("%d",&type);
        if (type==1)             //if H then blue
           type=19;
        else type=14;            //else C is red
        printf ("%s     %s     %s     %d\n", x,y,z,type);
        k++;
     }

     j=1;
```

```
   while (j<=192){                  //prints the second surface
      scanf("%s ",&x);
      scanf("%s ",&y);
      scanf("%s ",&z);
      scanf("%d",&type);
      printf ("%s     %s     %s     %d\n", x,y,z,type);
      j++;
   }
  if (i!=frames){                   //prints number of atoms in frame
   scanf ("%d",&atoms);
   printf("%d \n", atoms);
  }
  i++;
  }                                 //end of while loop
}                                   //end of program
```

```
//Author:  Catherine Manning
//Description:  This program converts from normal format to moviemol
//***************************************************************************

//***************************************************************************
//Libraries
#include<stdio.h>
#include<string.h>

#define MAXSTR 500
void convert ();

//***************************************************************************
int main (){

  char line[100],blank[4];      //line is the xyz
                                //blank is the type of atoms
  int  atomic[392];             //type of atoms
  int a,b,c,d,x,y,z,i,j;        //counters

  for (j=0;j<3;j++){            //gets first three lines
    fgets (line,MAXSTR,stdin);
  }

  for (c=0; c<394; c++)         //initialization
    atomic[c]=0;
  d=0;
  for (y=1; y<14; y++) {      //puts the correct atoms type into the array
    for (x=1; x<31; x++){
      scanf ("%d",&a);
      if (a==1)
        a=6;
      else
        a=1;
    atomic[d]=a;
   d++;

   }
  }

  for (i=1; i<3; i++){          //gets xyz coordinates
    scanf ("%d",&a);
    if (a==1)
      atomic[389+i]=8;
    else
      atomic[389+i]=1;
  }

fgets(line,MAXSTR,stdin);
z=0;
while (z<392){                  //prints the final result
  fgets(blank,3,stdin);
  fgets(line, 100, stdin);
  line[strlen(line)-1]=0;
  z++;
  printf("%s %d\n",line,atomic[z]);


 }
```

Ethane Molecule Between Surfaces

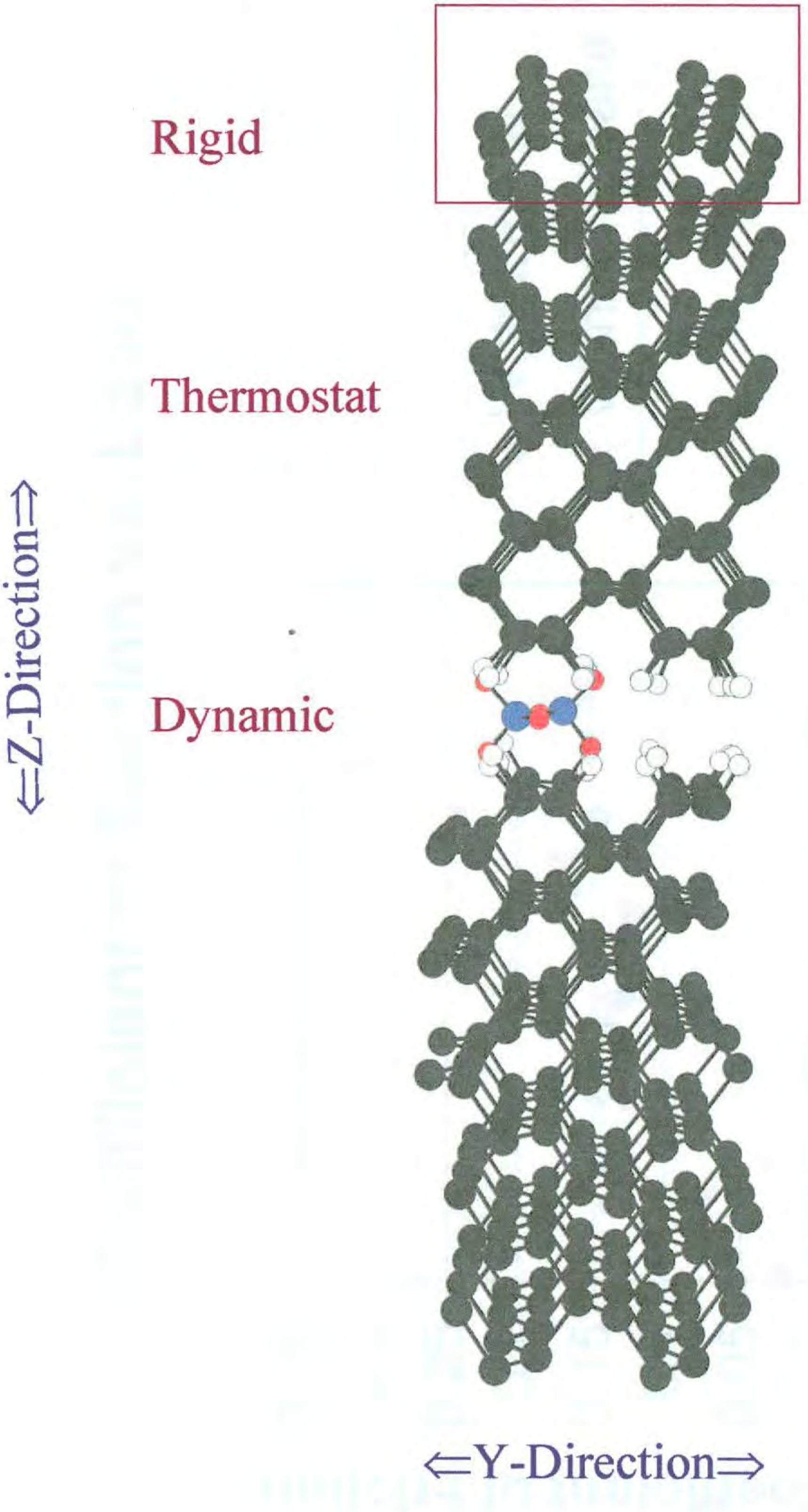


Figure 1

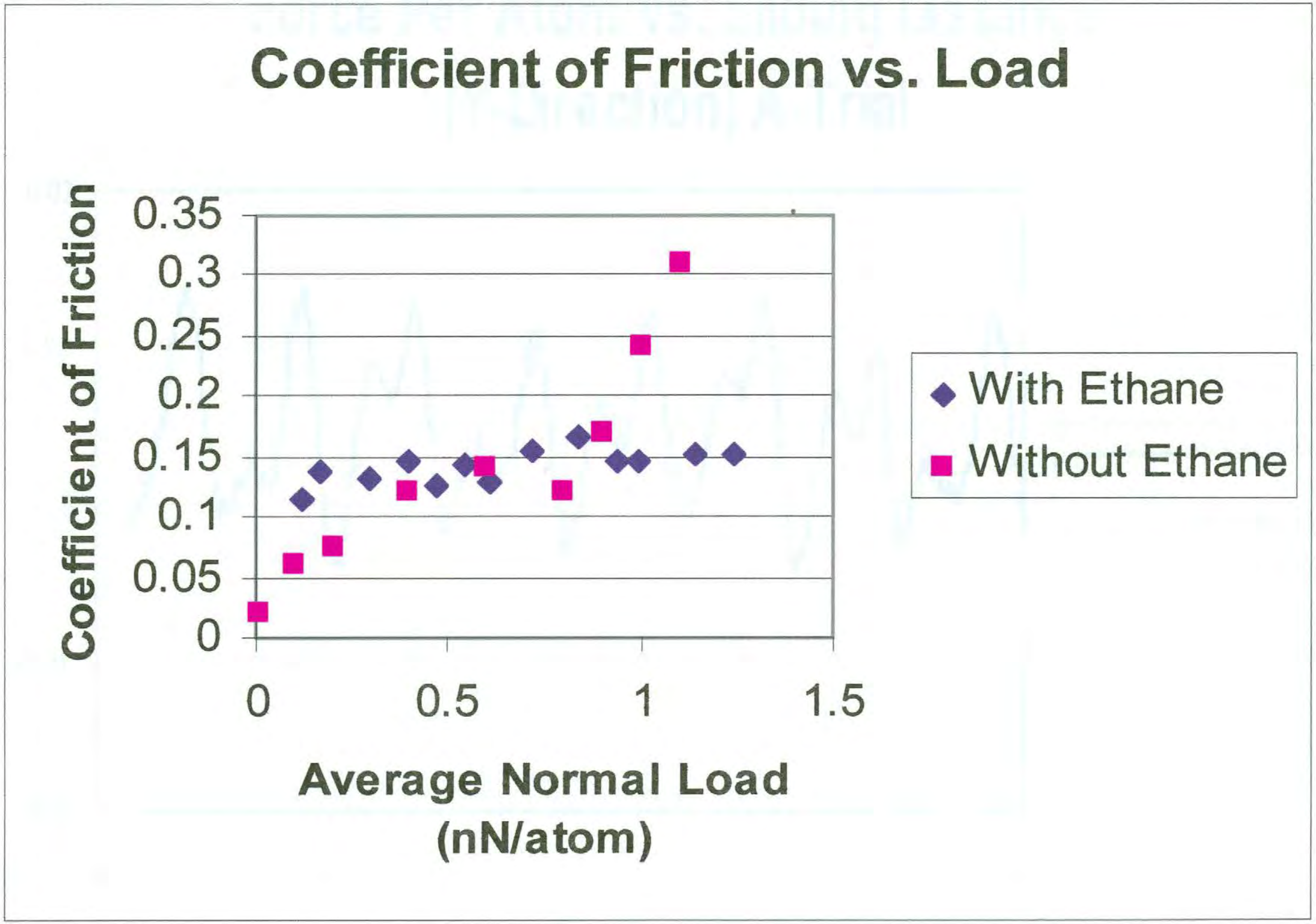

Coefficient of Friction vs. Load
Coefficient of Friction
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
0.5
1
1.5
Average Normal Load (nN/atom)
◆ With Ethane
■ Without Ethane

Figure 2

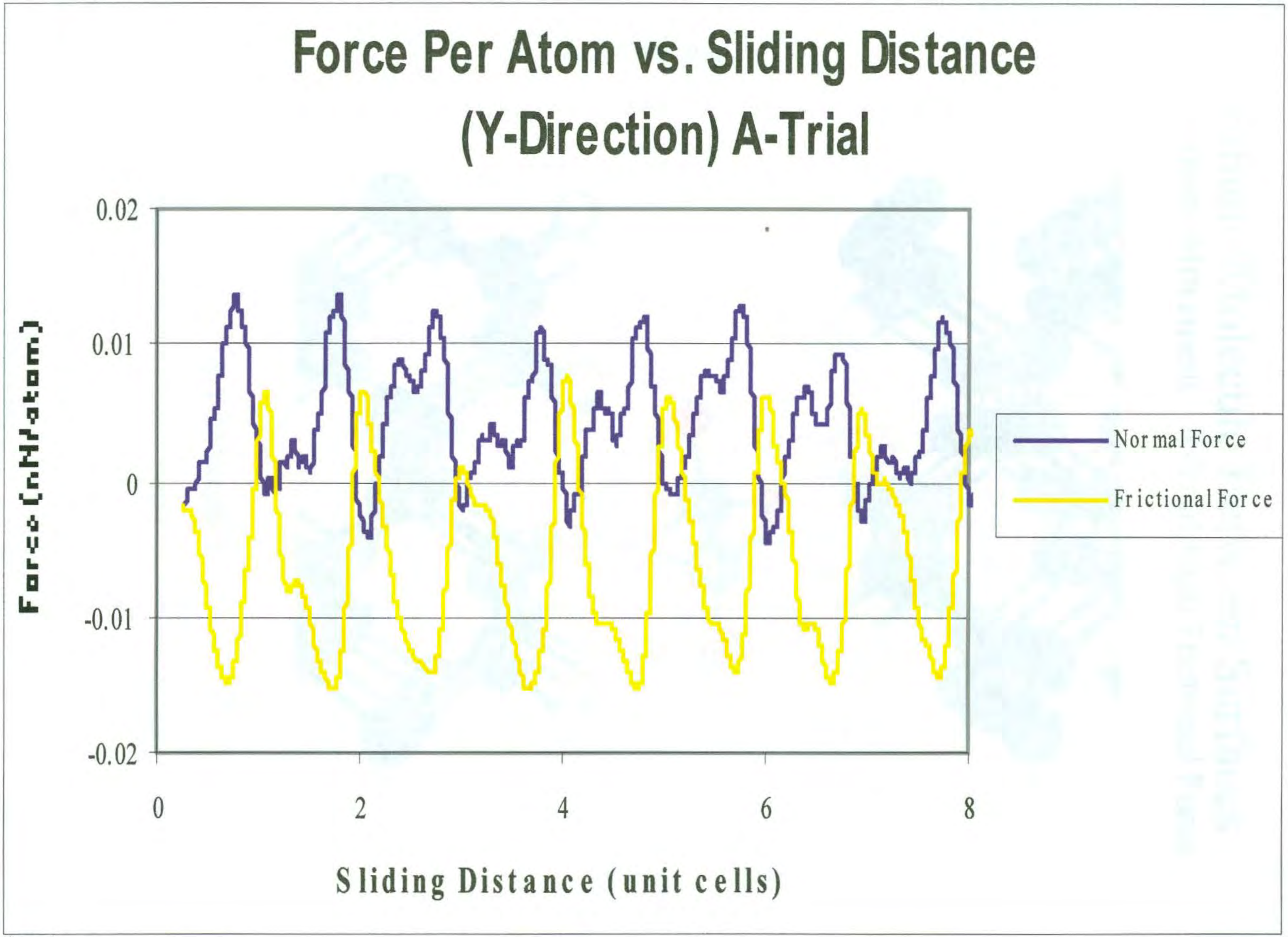

Force Per Atom vs. Sliding Distance (Y-Direction) A-Trial
0.02
0.01
0
-0.01
-0.02
Force (nN/atom)
0
2
4
6
8
Sliding Distance (unit cells)
Normal Force
Frictional Force

Figure 3

Ethane Molecule Between Surfaces

Ethane Movement - A-Trial Low Frictional Force

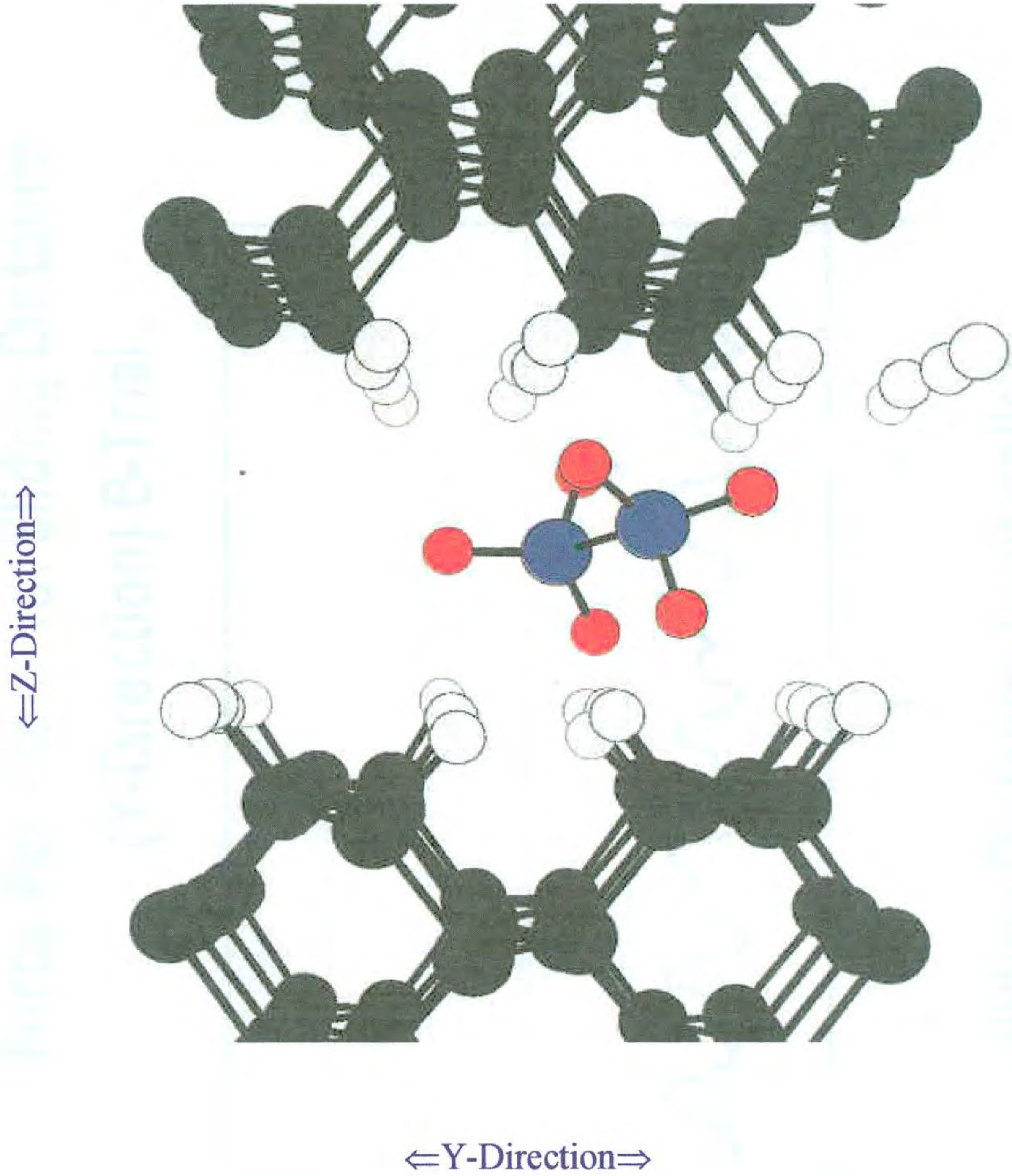


Figure 5


Force Per Atom vs. Sliding Distance (Y-Direction) B-Trial
0.1
0.08
0.06
0.04
0.02
0
-0.02
Force (nN/atom)
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 6

Ethane Molecule Between Surfaces

Ethane Movement - B-Trial High Frictional Force

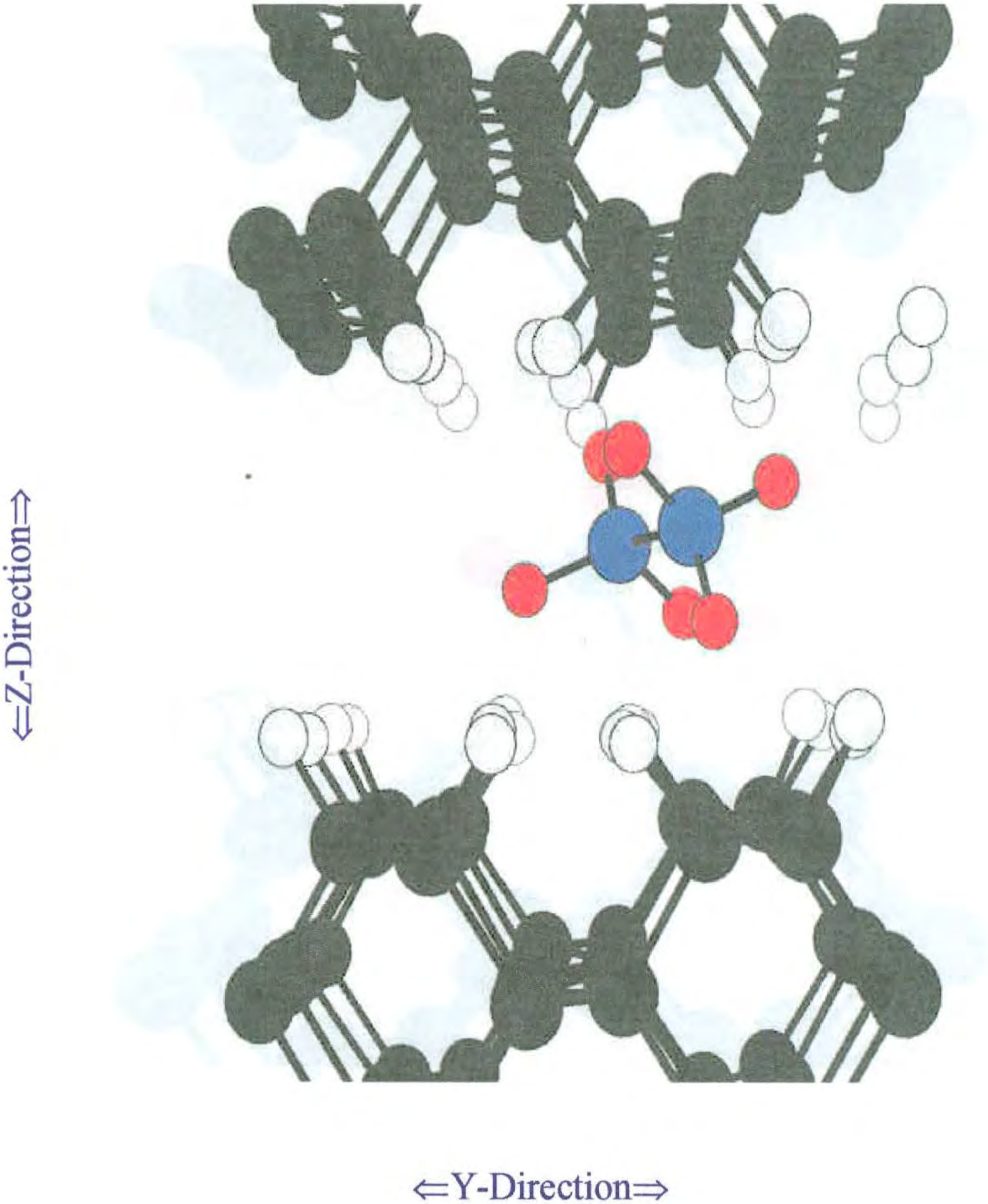


Figure 7

Ethane Molecule Between Surfaces

Ethane Movement - B-Trial Low Frictional Force

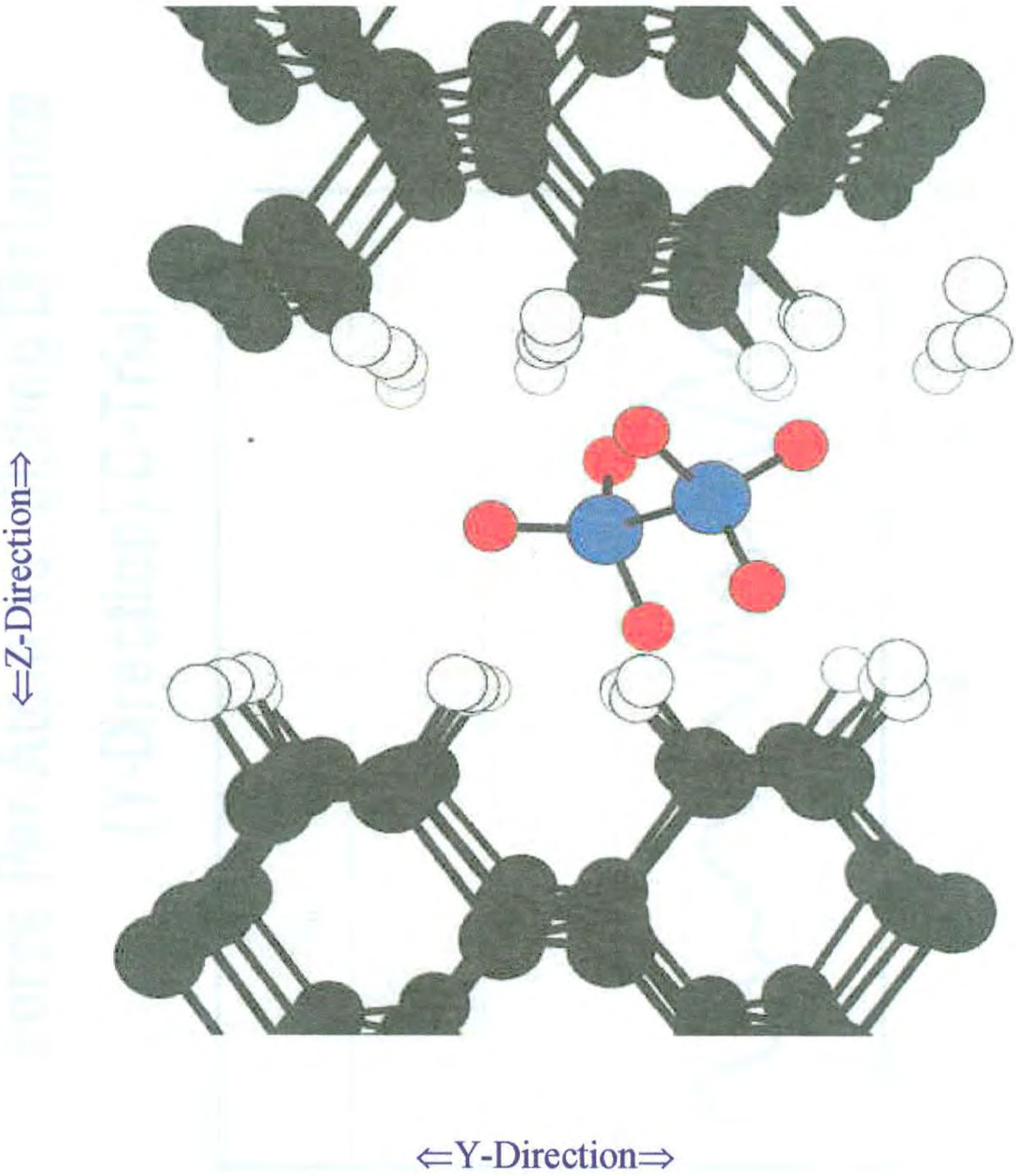


Figure 8

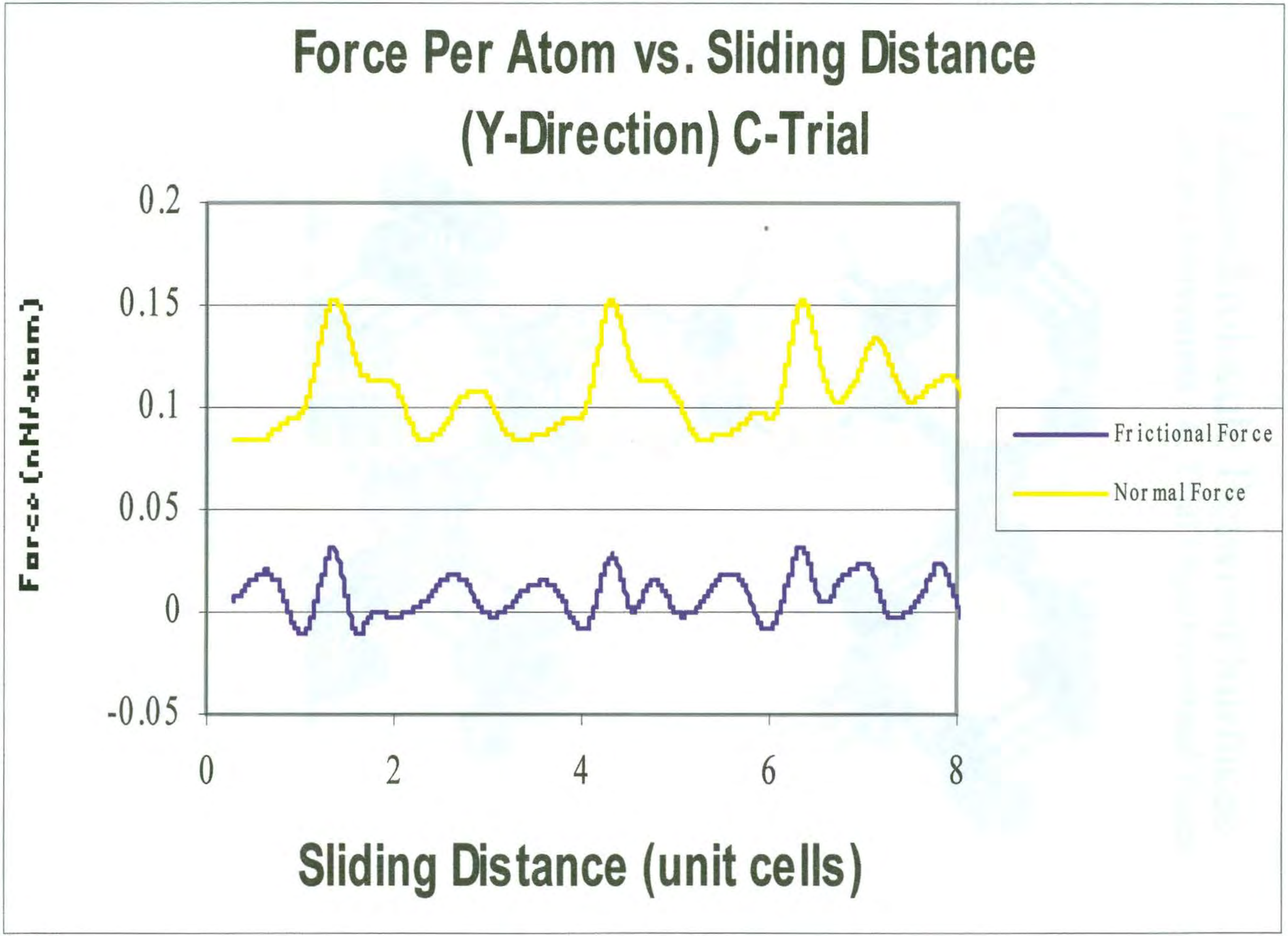

Force Per Atom vs. Sliding Distance (Y-Direction) C-Trial
Force (nN/atom)
0.2
0.15
0.1
0.05
0
-0.05
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 9

Ethane Molecule Between Surfaces

Ethane Movement - C-Trial High Frictional Force

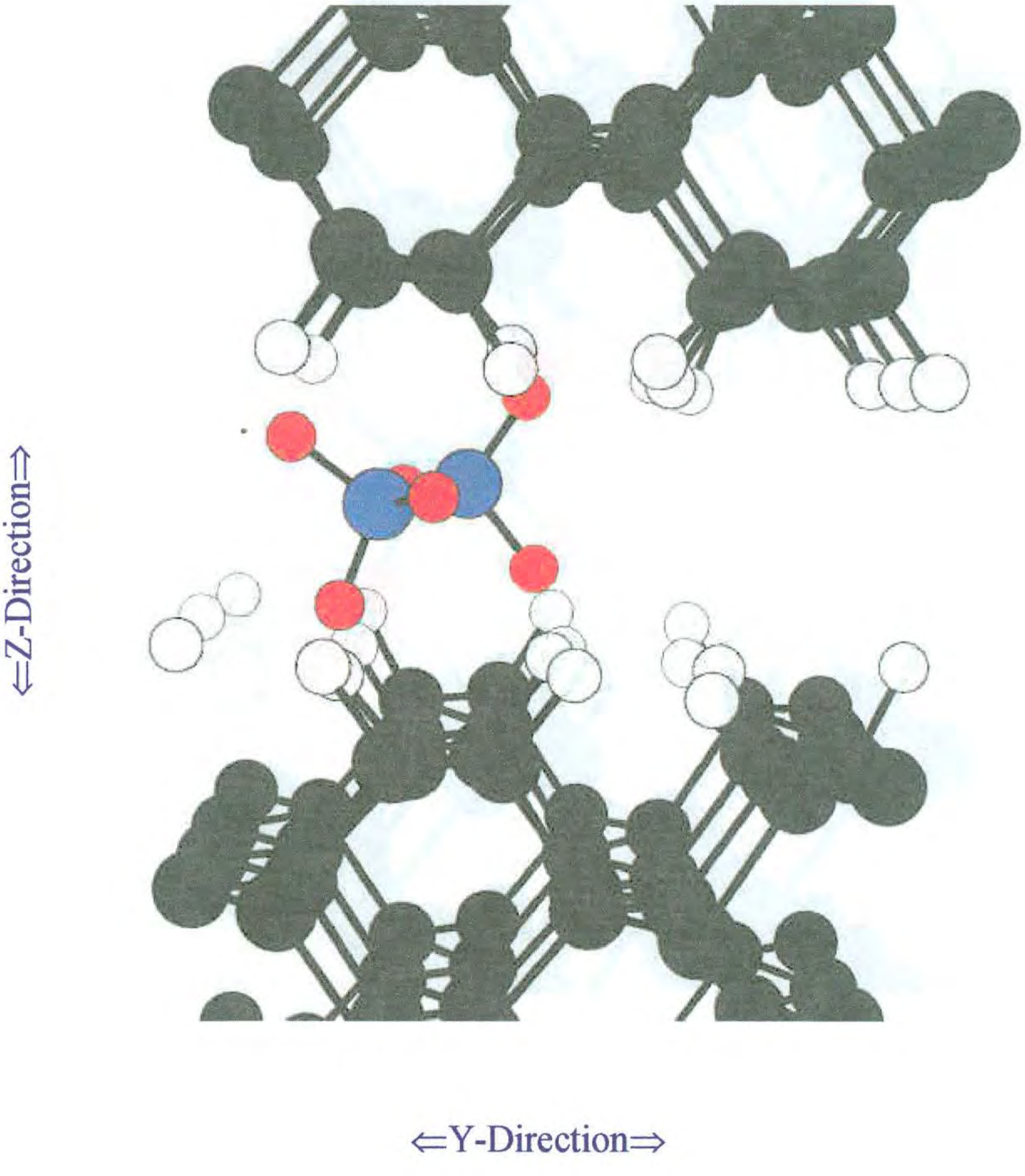


Figure 10

Ethane Molecule Between Surfaces

Ethane Movement - C-Trial Low Frictional Force

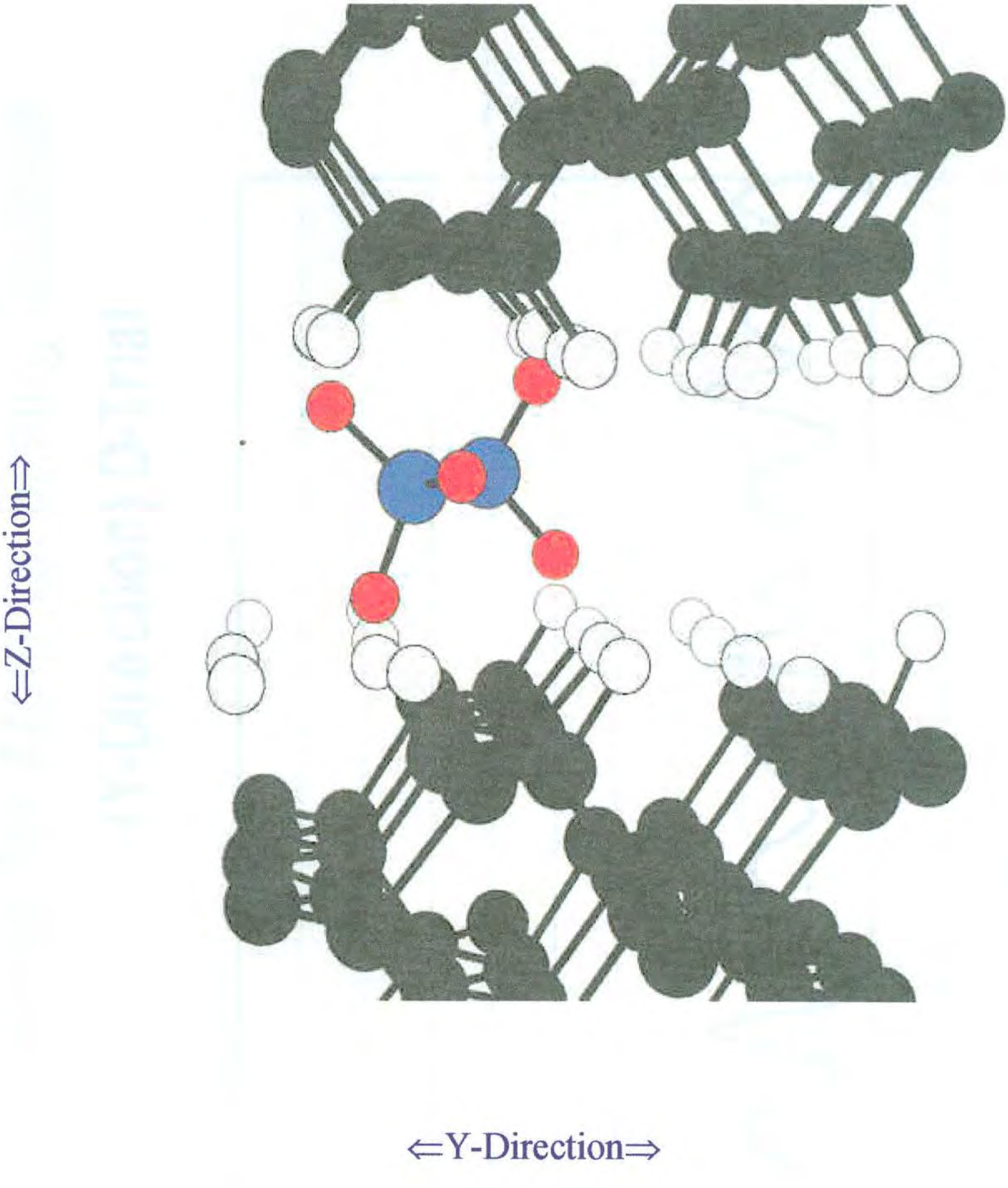


Figure 11

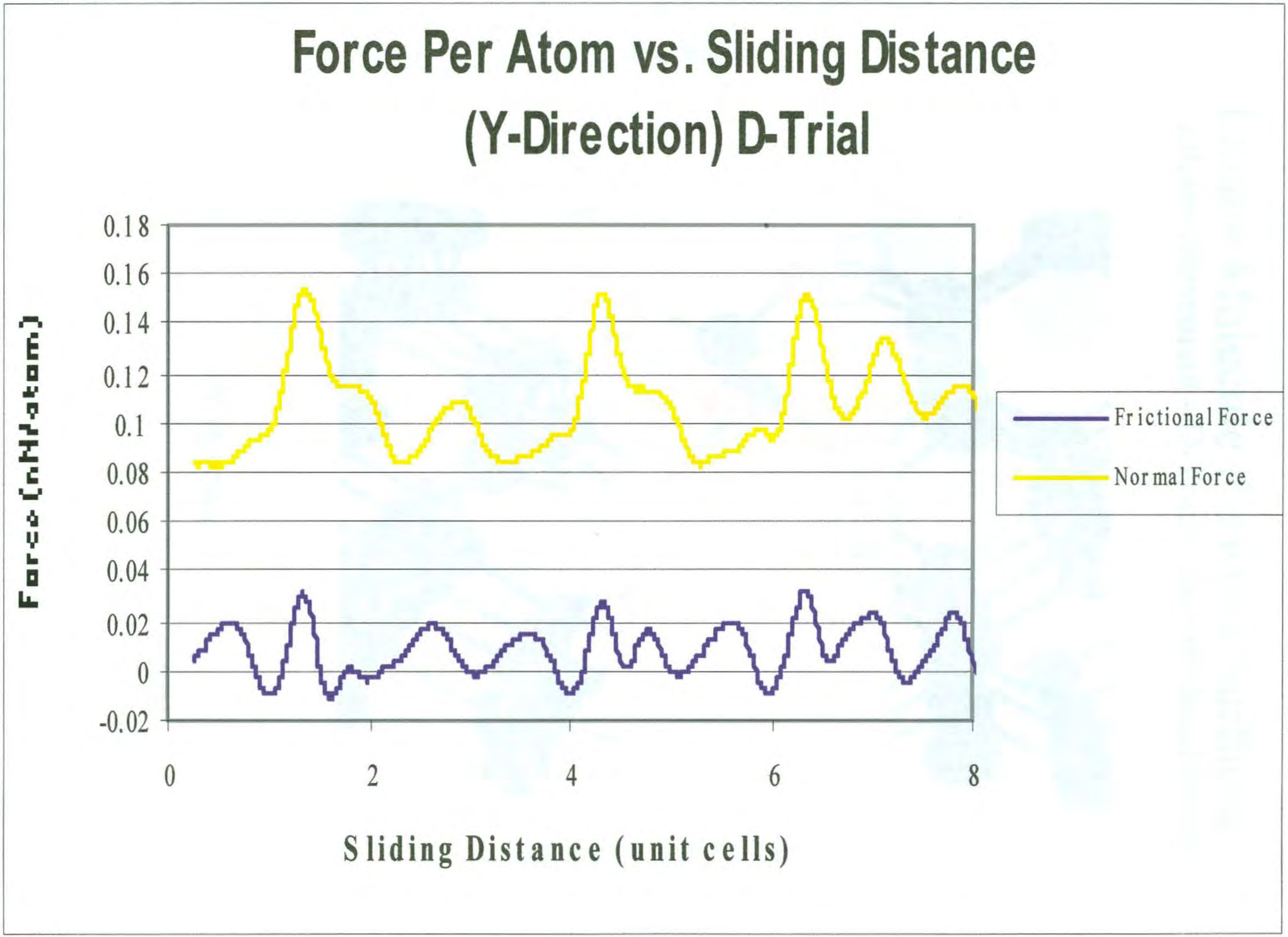

Force Per Atom vs. Sliding Distance
(Y-Direction) D-Trial
Force (nN/atom)
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
-0.02
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 12

Ethane Molecule Between Surfaces

Ethane Movement - D-Trial Low Frictional Force

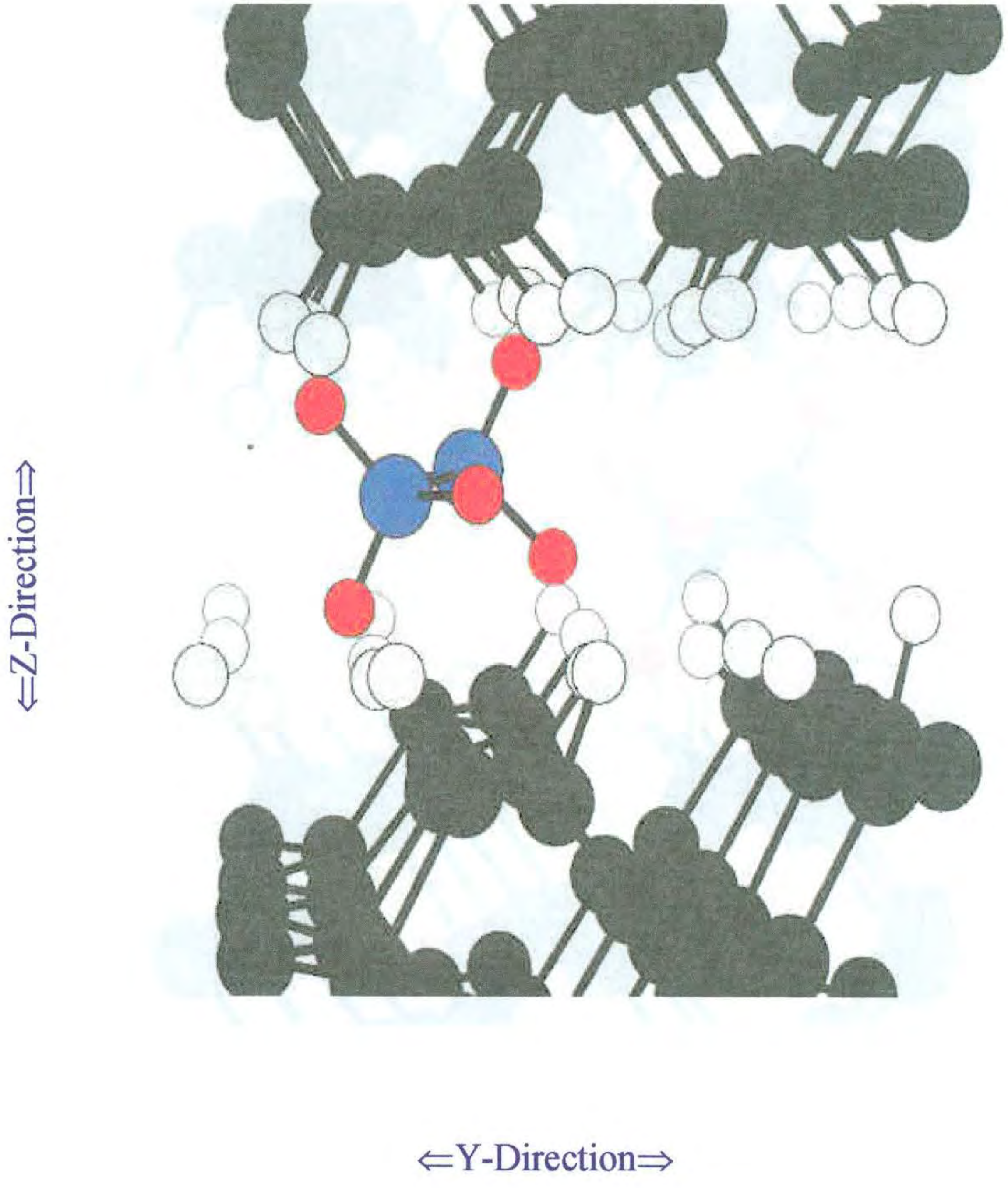


Figure 13

Ethane Molecule Between Surfaces

Ethane Movement - D-Trial High Frictional Force

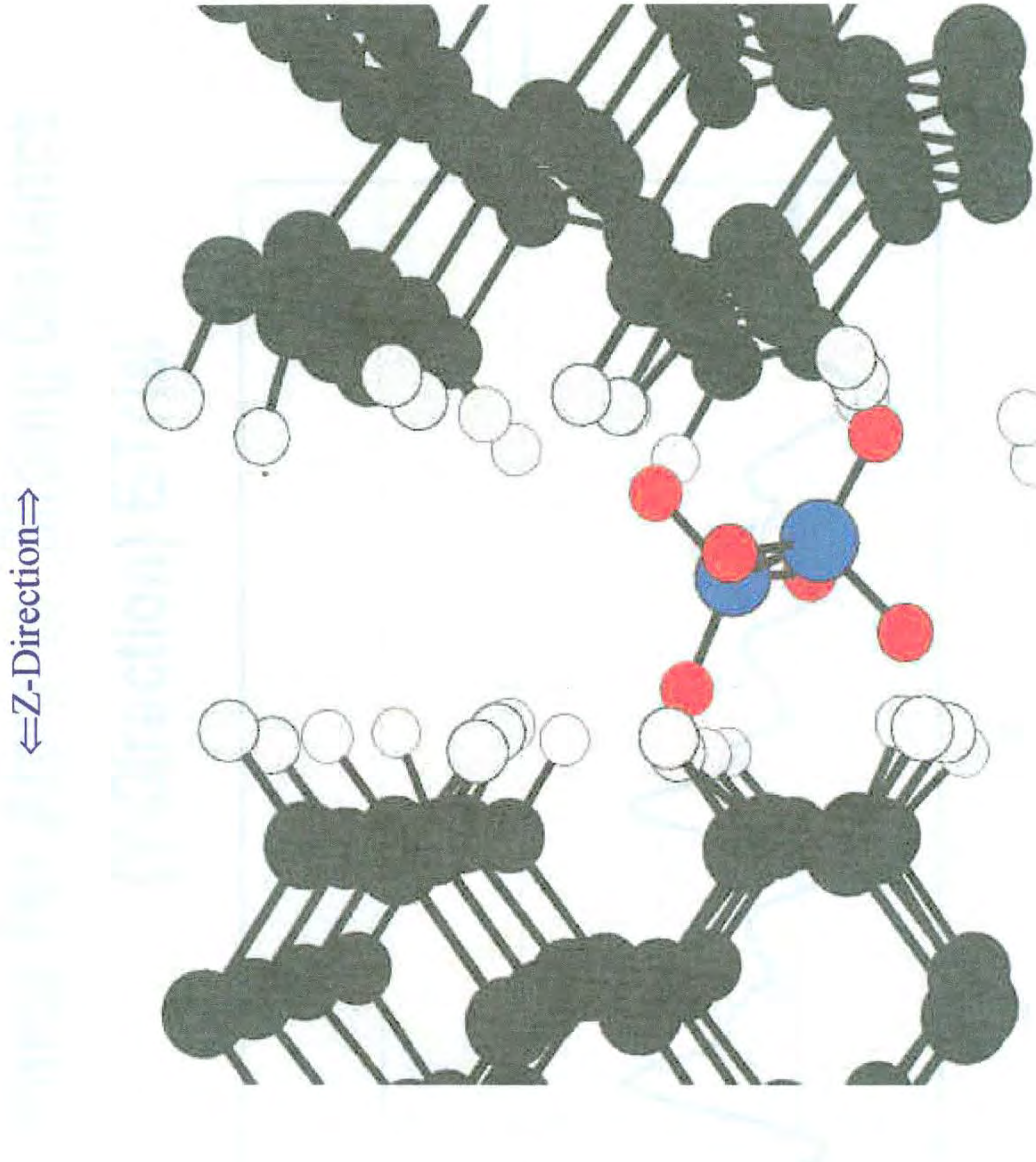


Figure 14


Force Per Atom vs. Sliding Distance (Y-Direction) E-Trial
Force (nN/atom)
0.2
0.15
0.1
0.05
0
-0.05
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 15

Ethane Molecule Between Surfaces

Ethane Movement - E-Trial High Frictional Force

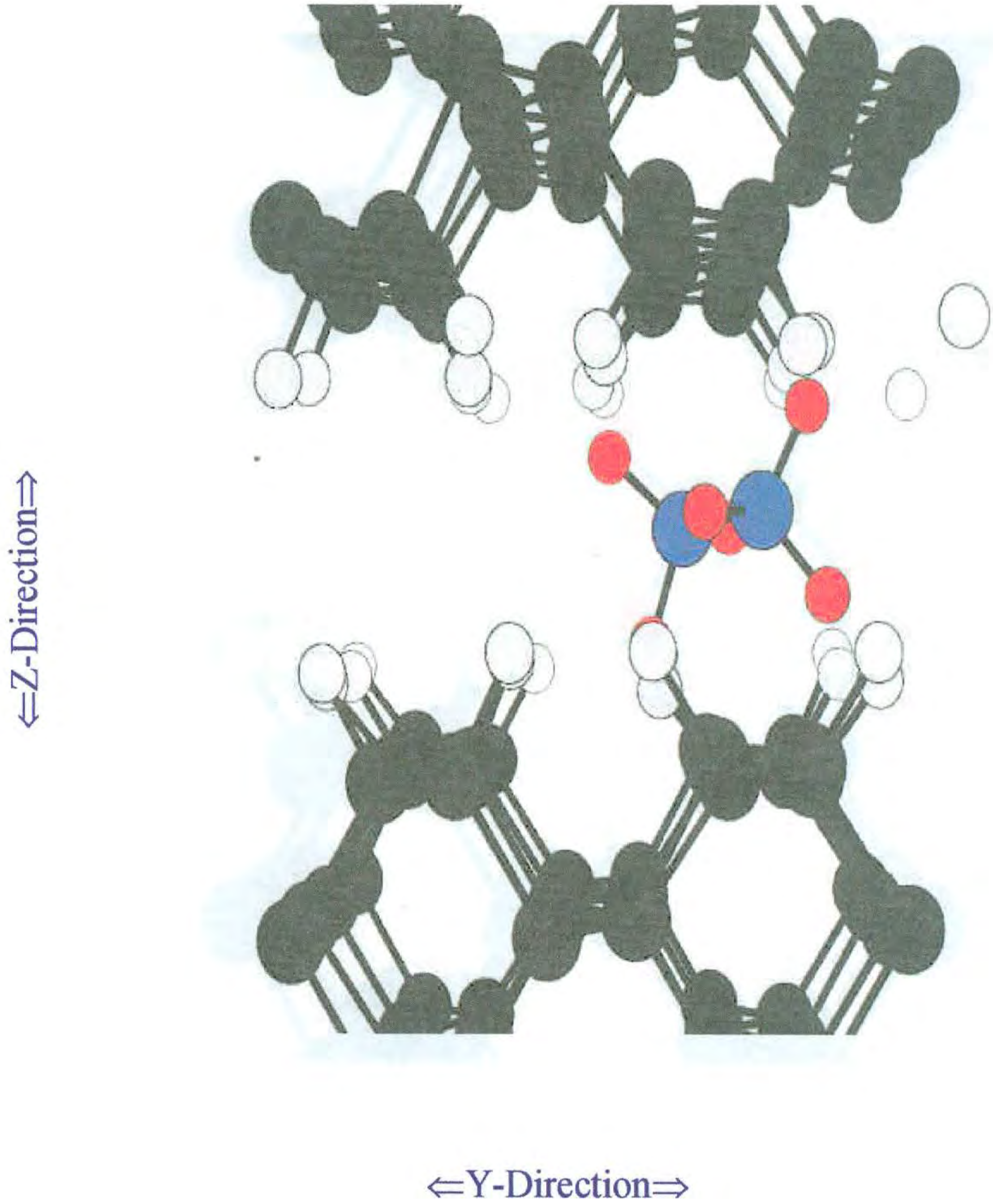


Figure 16

Ethane Molecule Between Surfaces

Ethane Movement - E-Trial Low Frictional Force

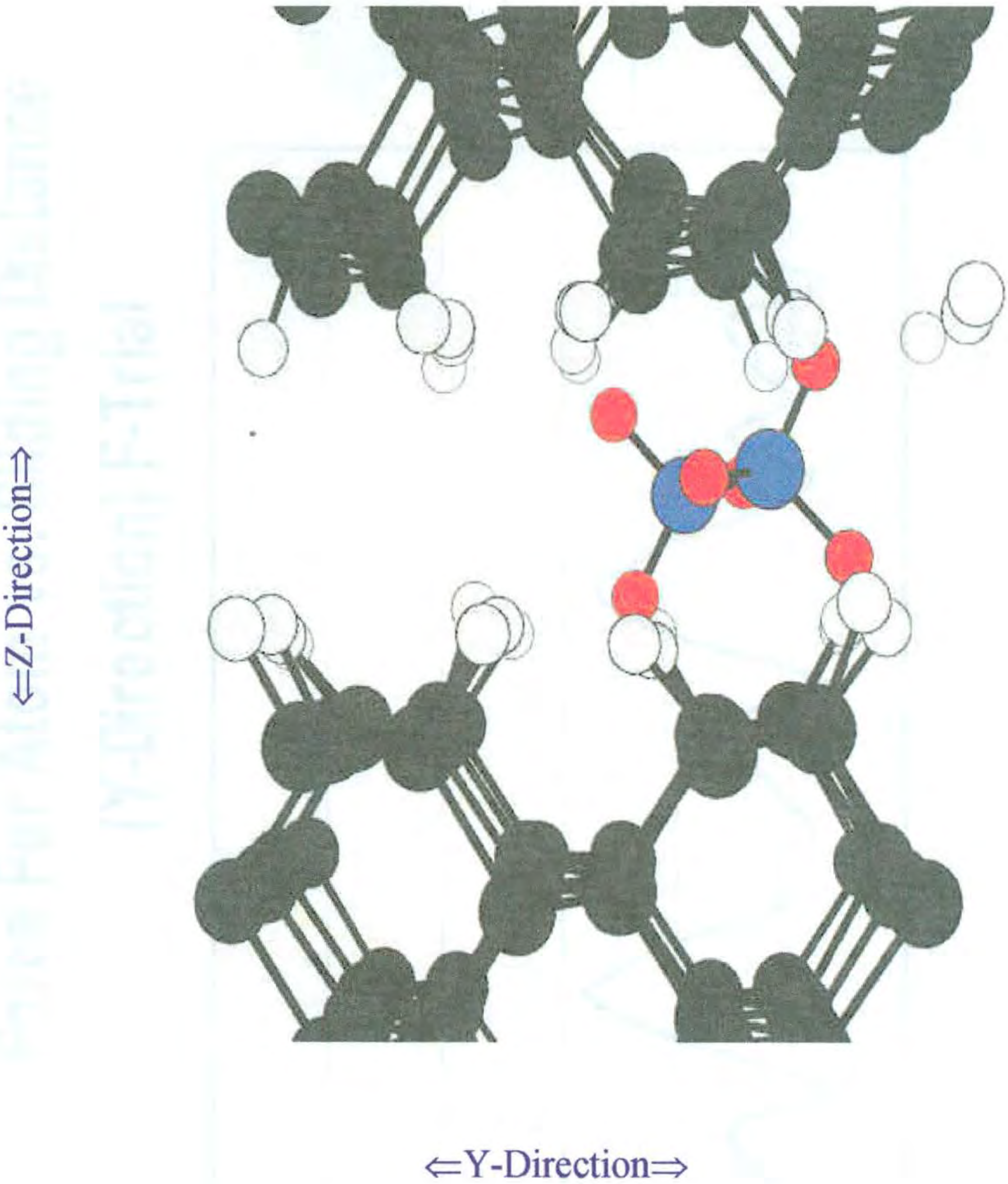


Figure 17

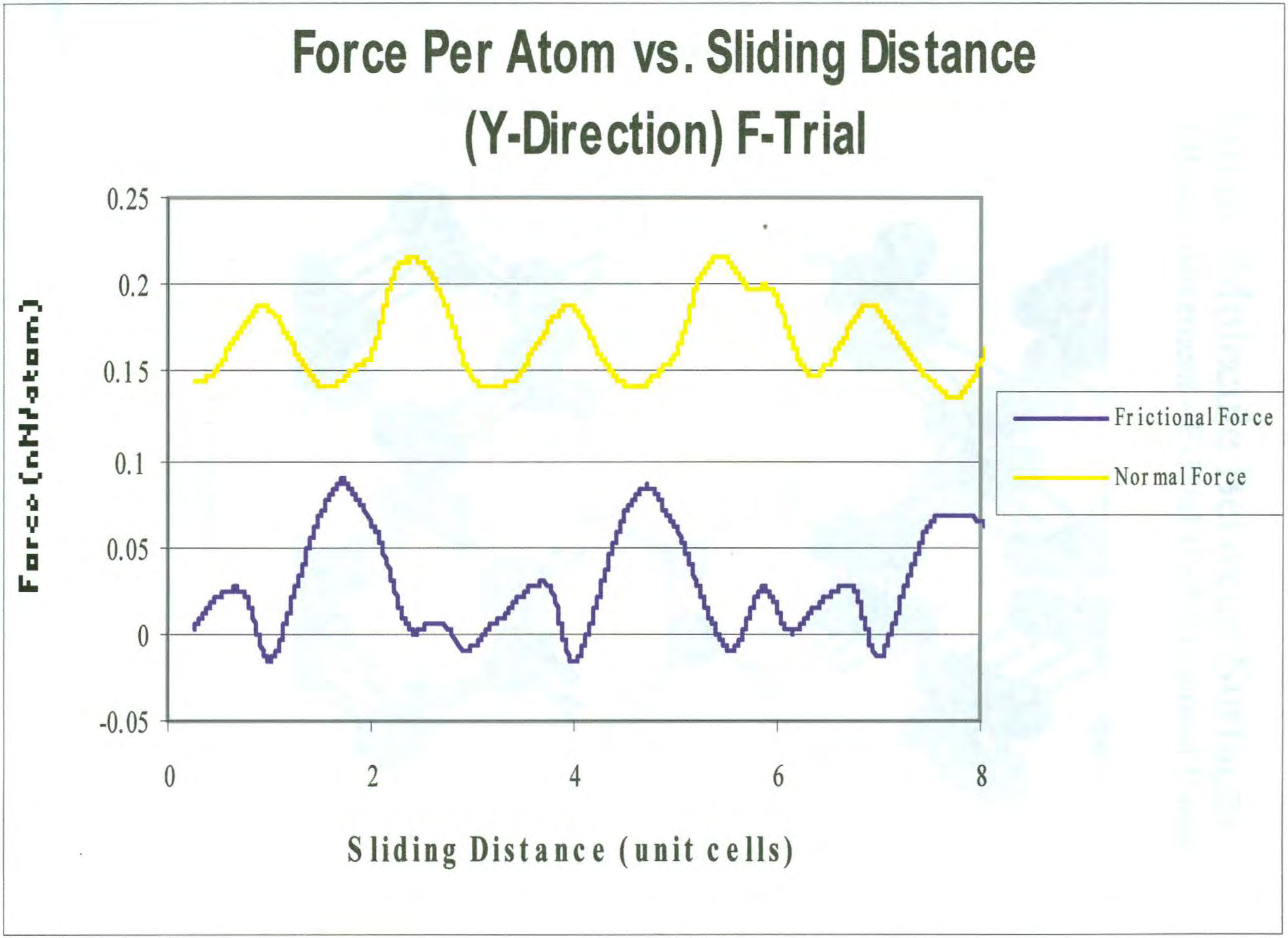

Force Per Atom vs. Sliding Distance (Y-Direction) F-Trial
Force (nN/atom)
0.25
0.2
0.15
0.1
0.05
0
-0.05
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 18

Ethane Molecule Between Surfaces

Ethane Movement - F-Trial High Frictional Force

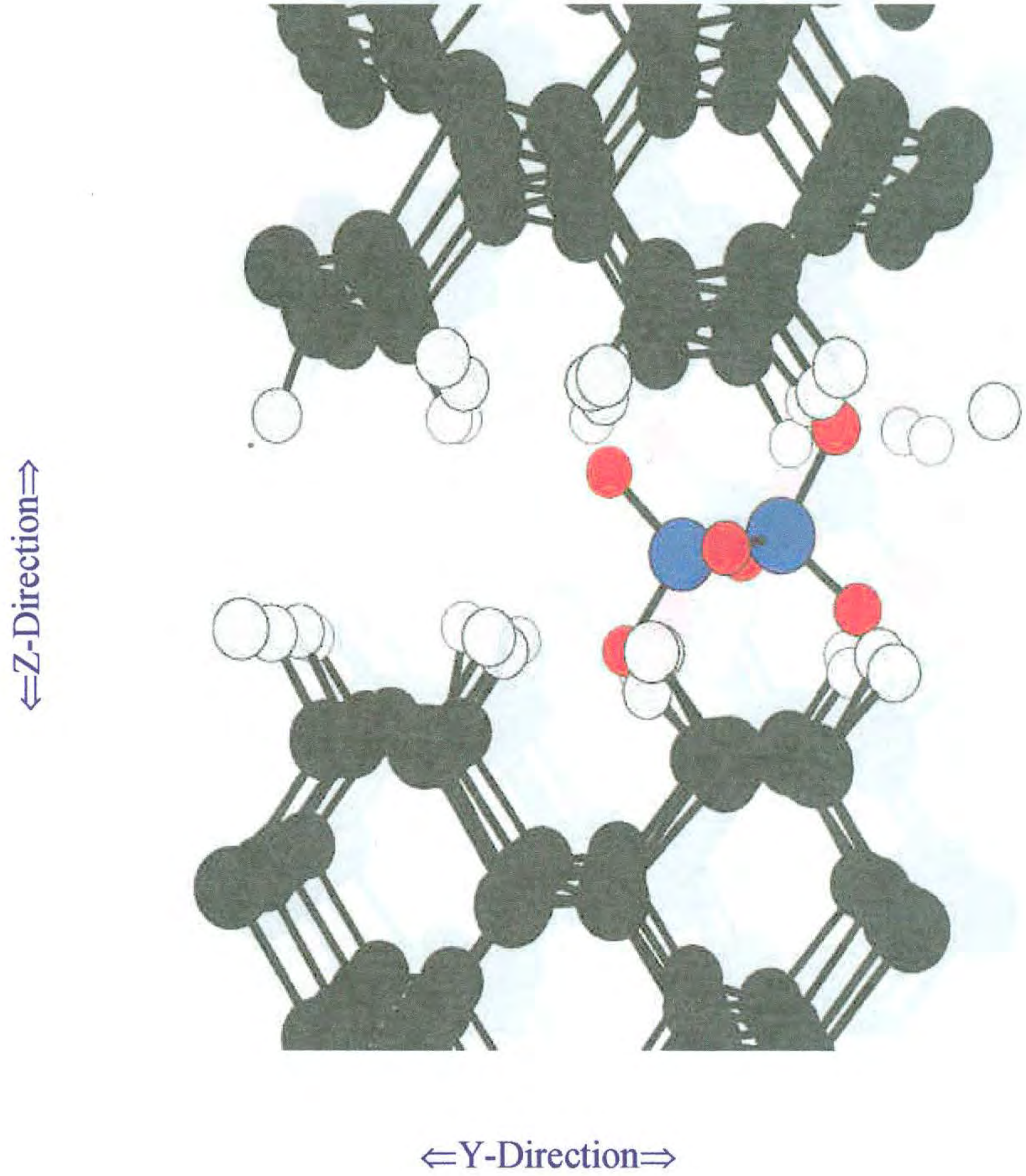


Figure 19

Ethane Molecule Between Surfaces

Ethane Movement - F-Trial Low Frictional Force

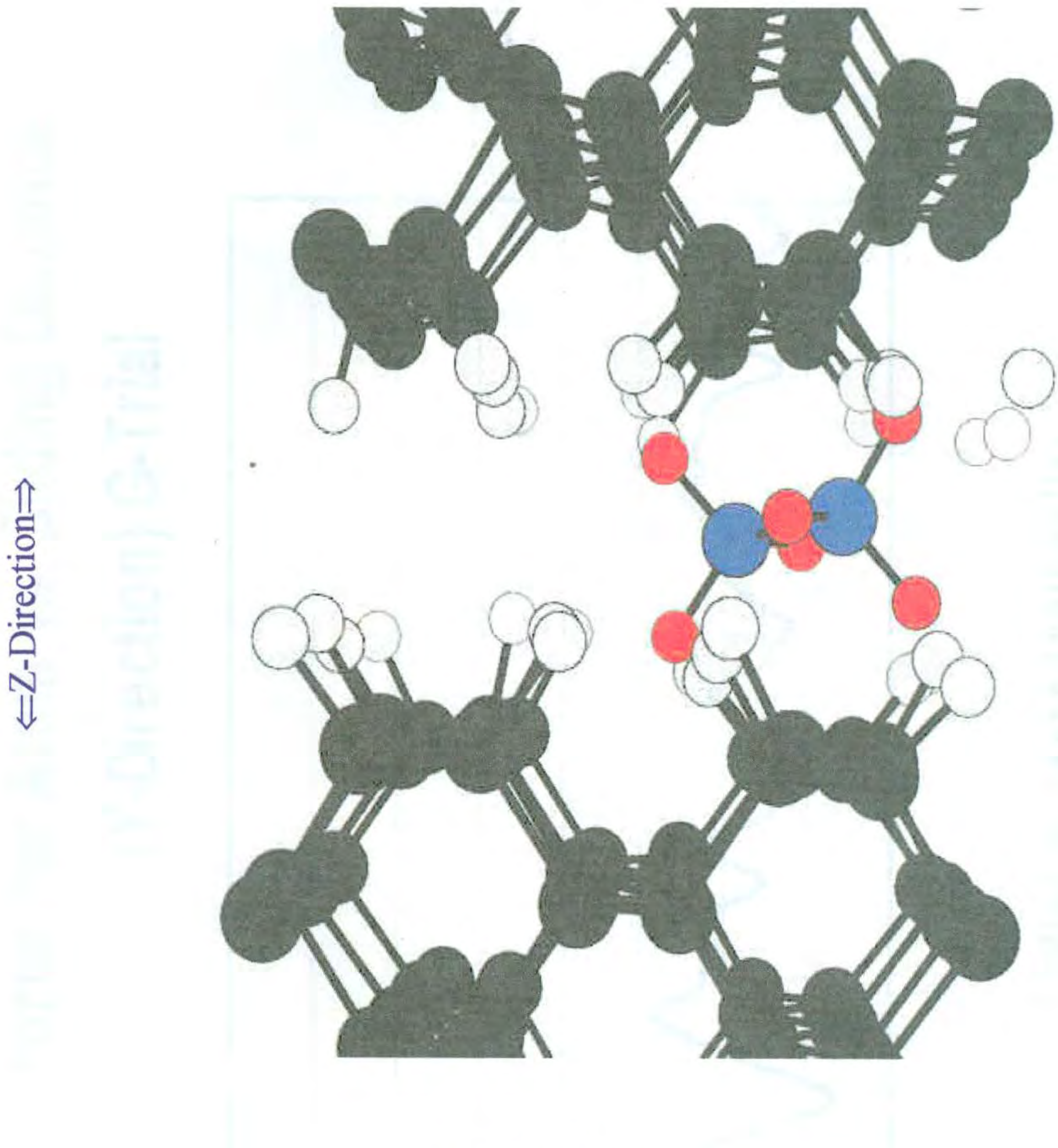


Figure 20

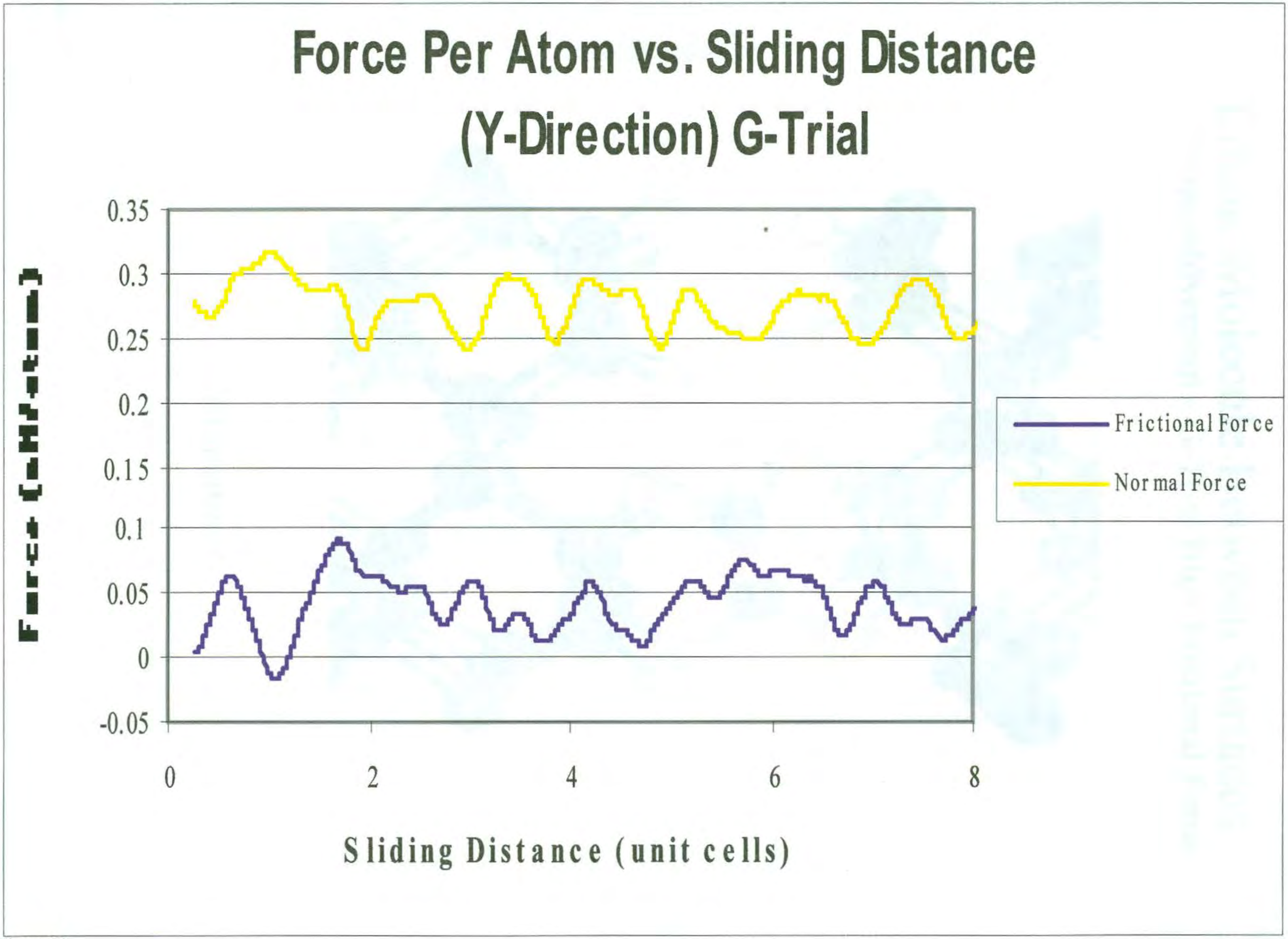

Force Per Atom vs. Sliding Distance (Y-Direction) G-Trial
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
0
2
4
6
8
Force
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 21

Ethane Molecule Between Surfaces

Ethane Movement - G-Trial High Frictional Force

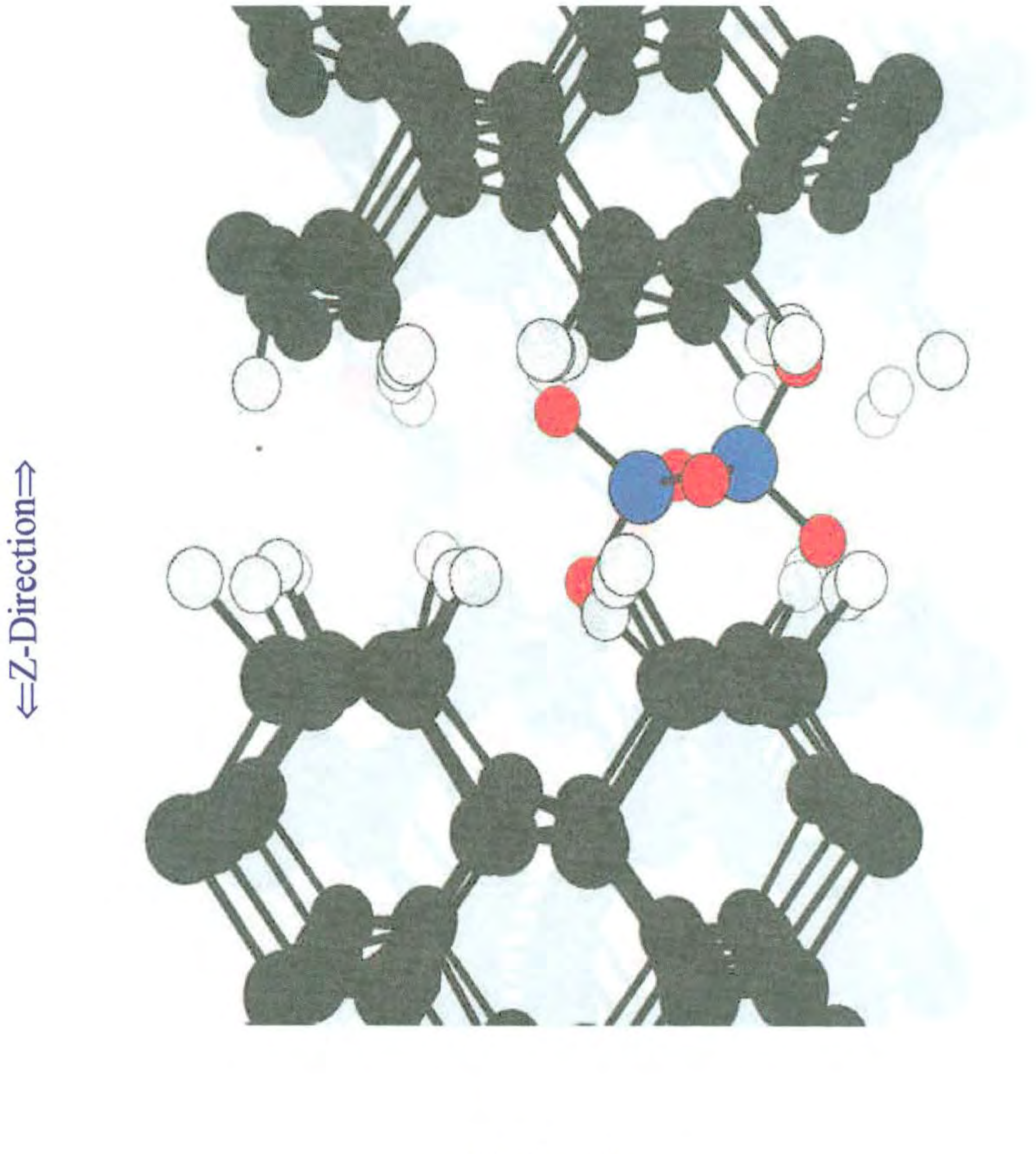


Figure 22

Ethane Molecule Between Surfaces

Ethane Movement - G-Trial Low Frictional Force

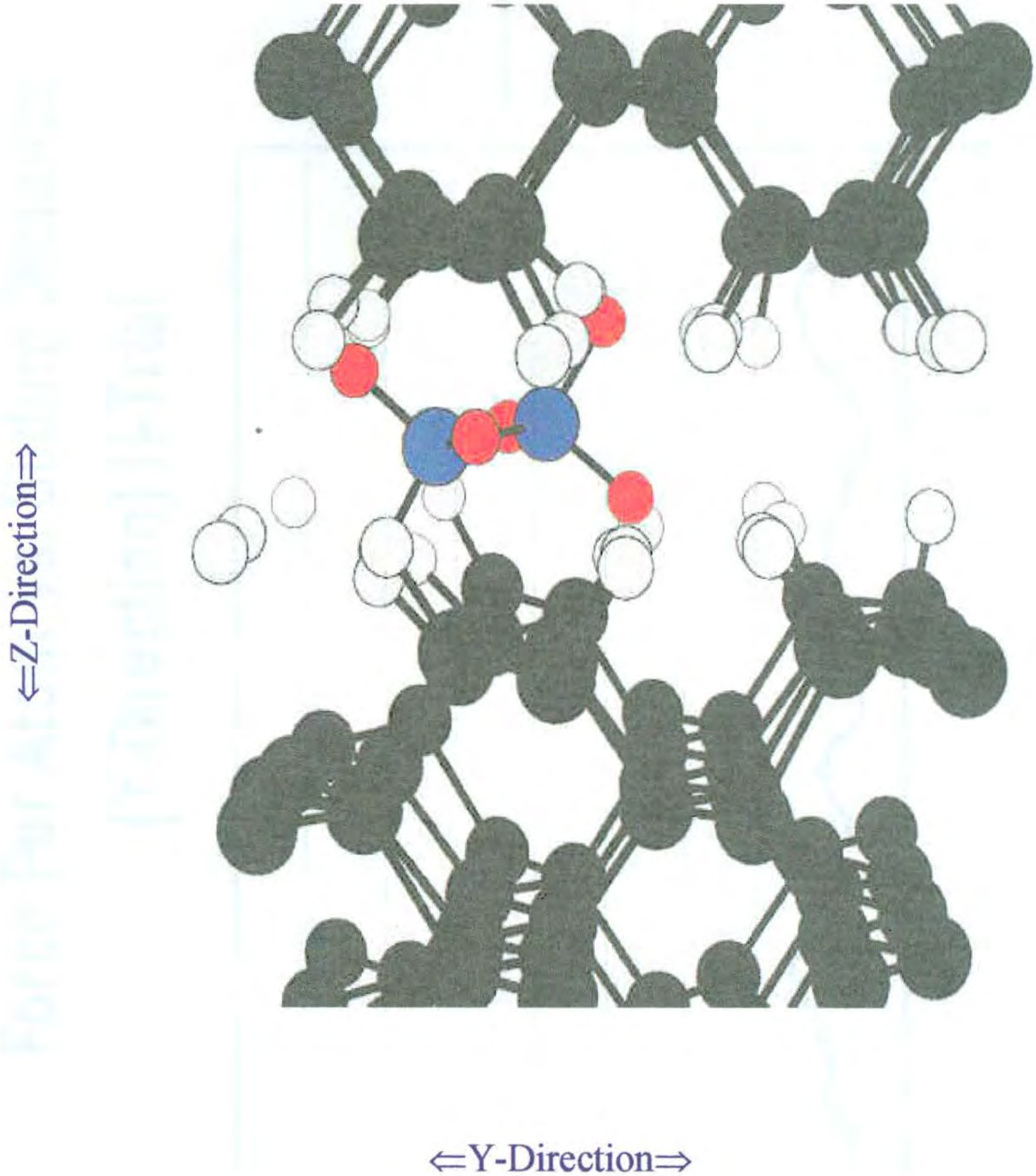


Figure 23

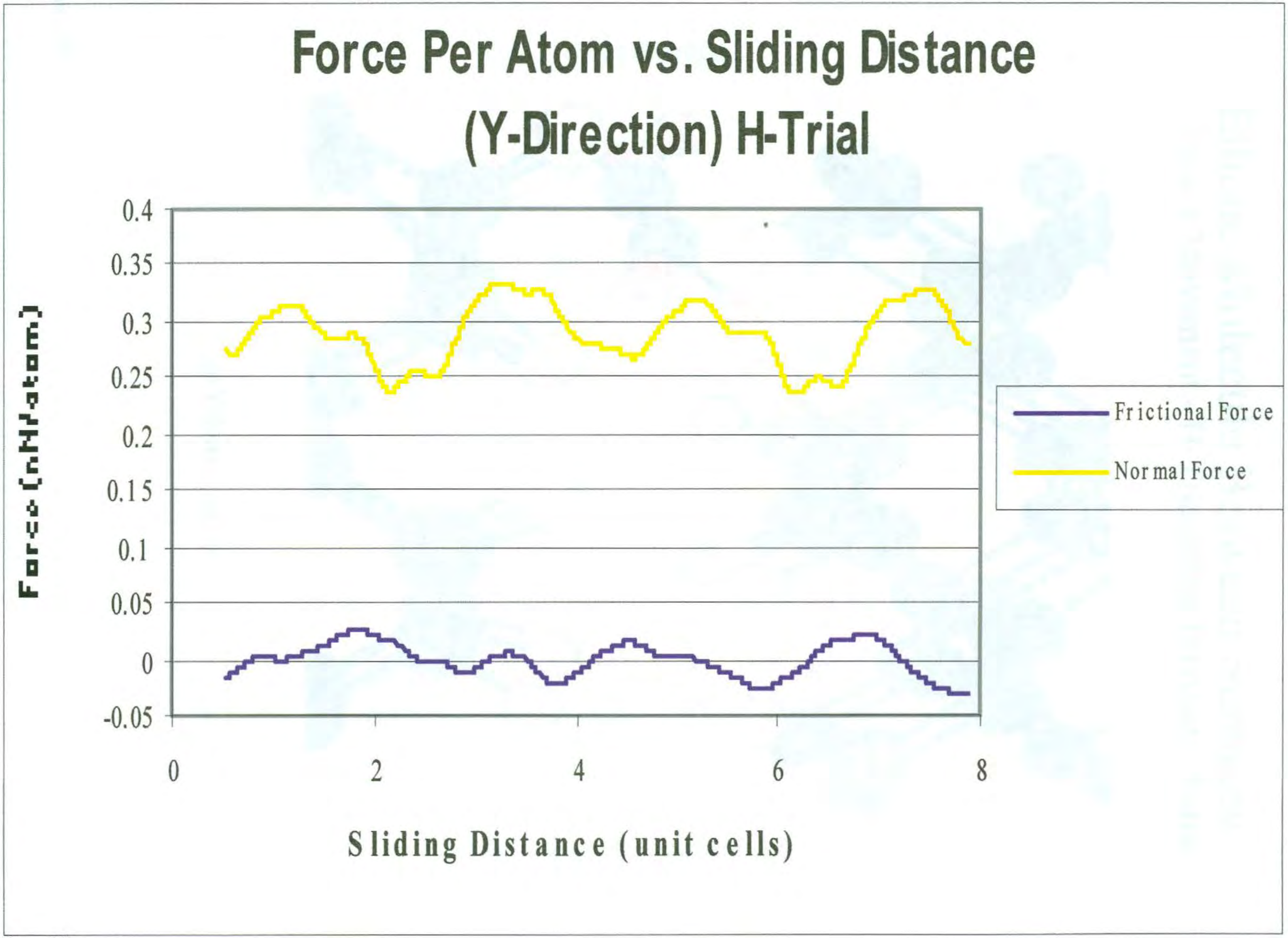

Force Per Atom vs. Sliding Distance (Y-Direction) H-Trial
Force (nN/atom)
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 24

Ethane Molecule Between Surfaces

Ethane Movement - H-Trial High Frictional Force

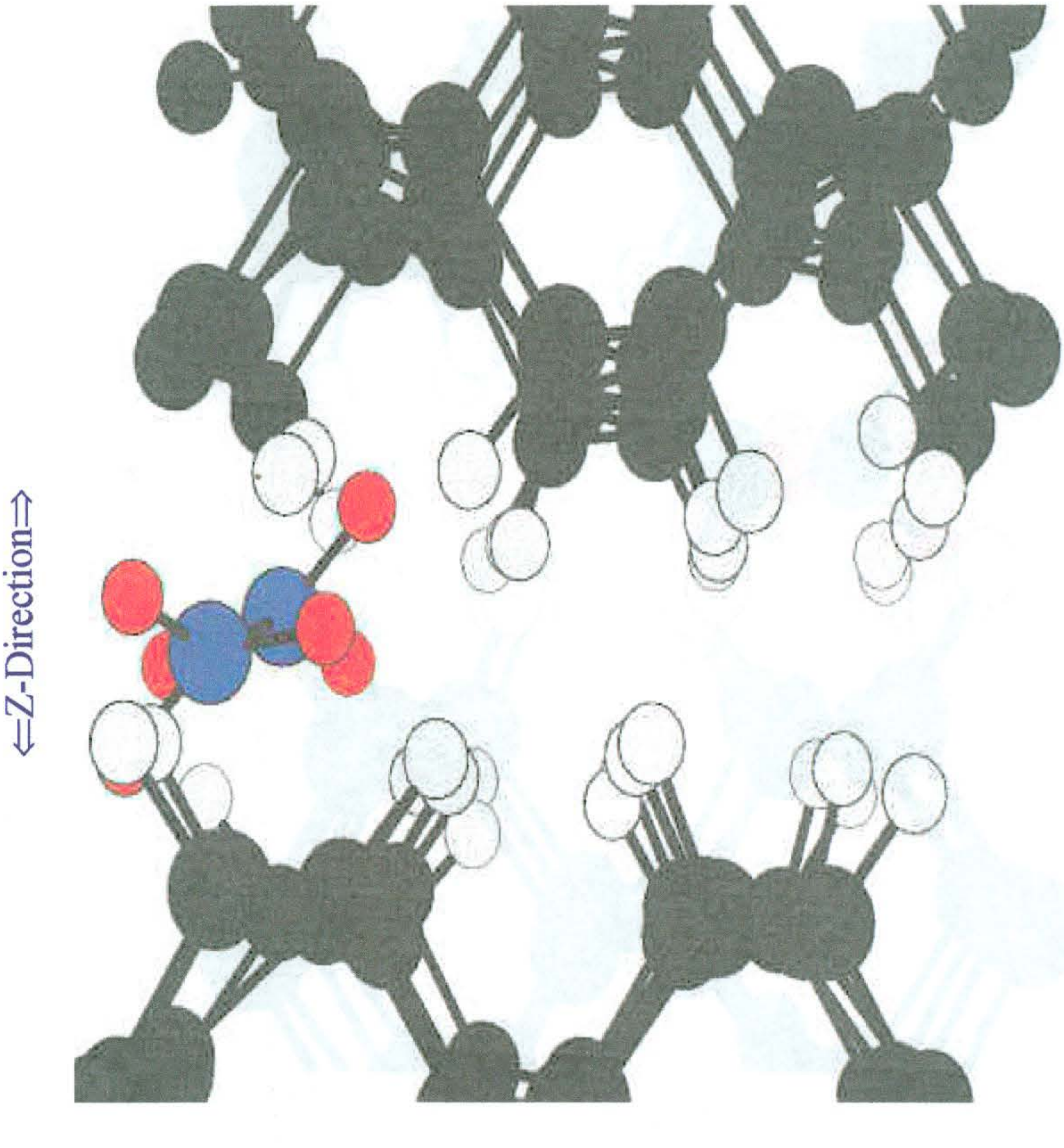


Figure 25

Ethane Molecule Between Surfaces

Ethane Movement - H-Trial Low Frictional Force

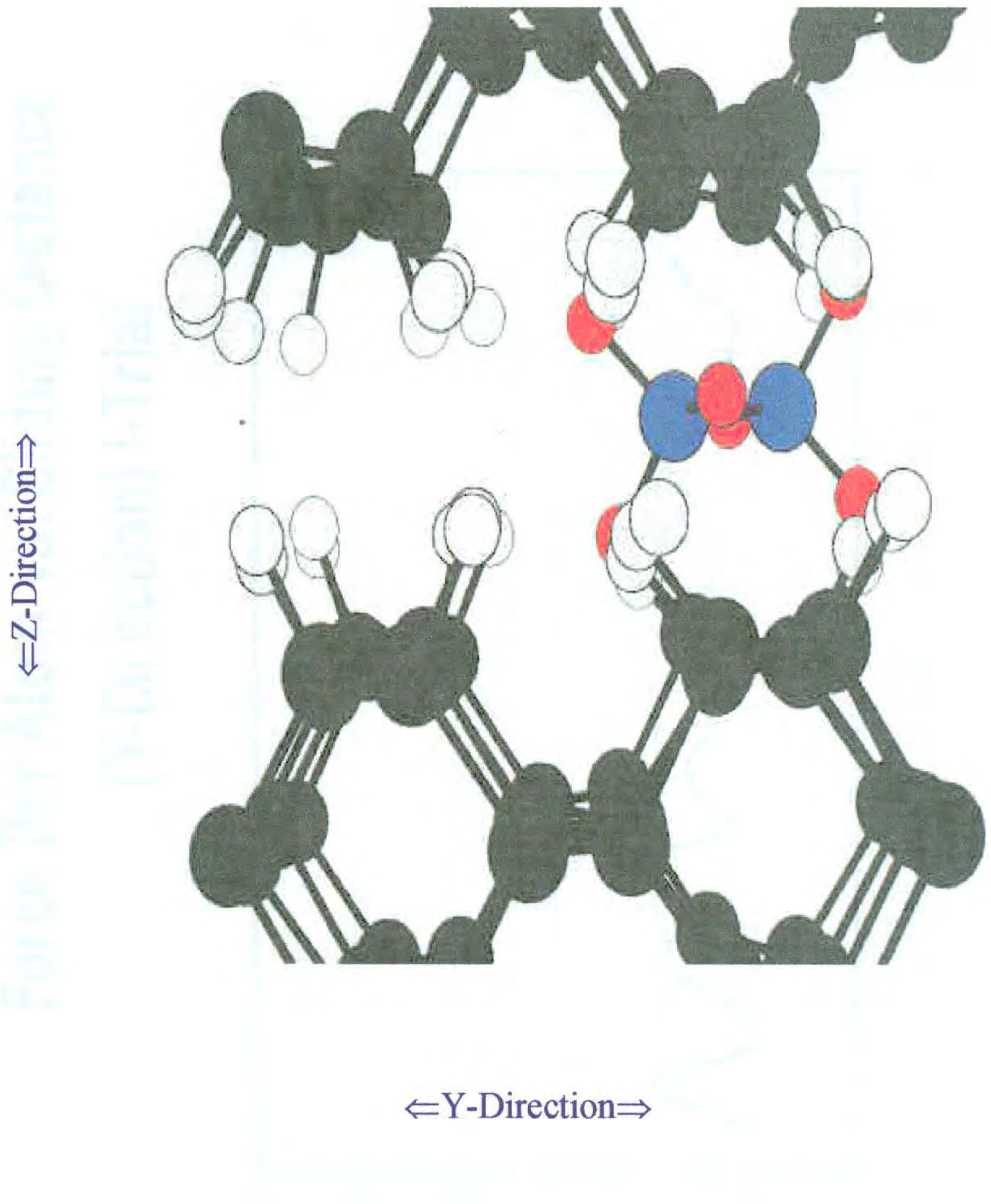


Figure 26

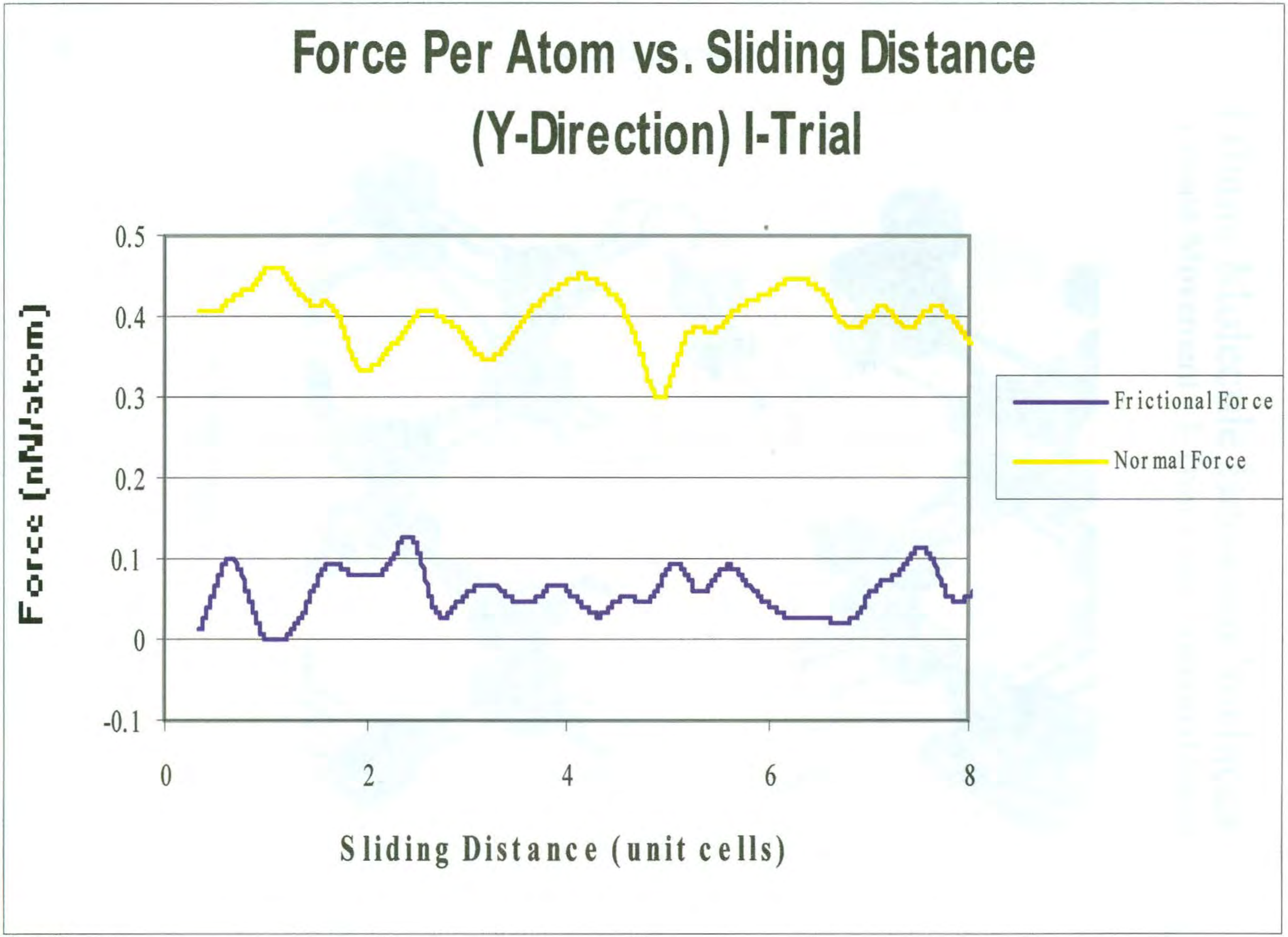

Force Per Atom vs. Sliding Distance (Y-Direction) I-Trial
Force (nN/atom)
0.5
0.4
0.3
0.2
0.1
0
-0.1
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 27

Ethane Molecule Between Surfaces

Ethane Movement - I-Trial High Frictional Force

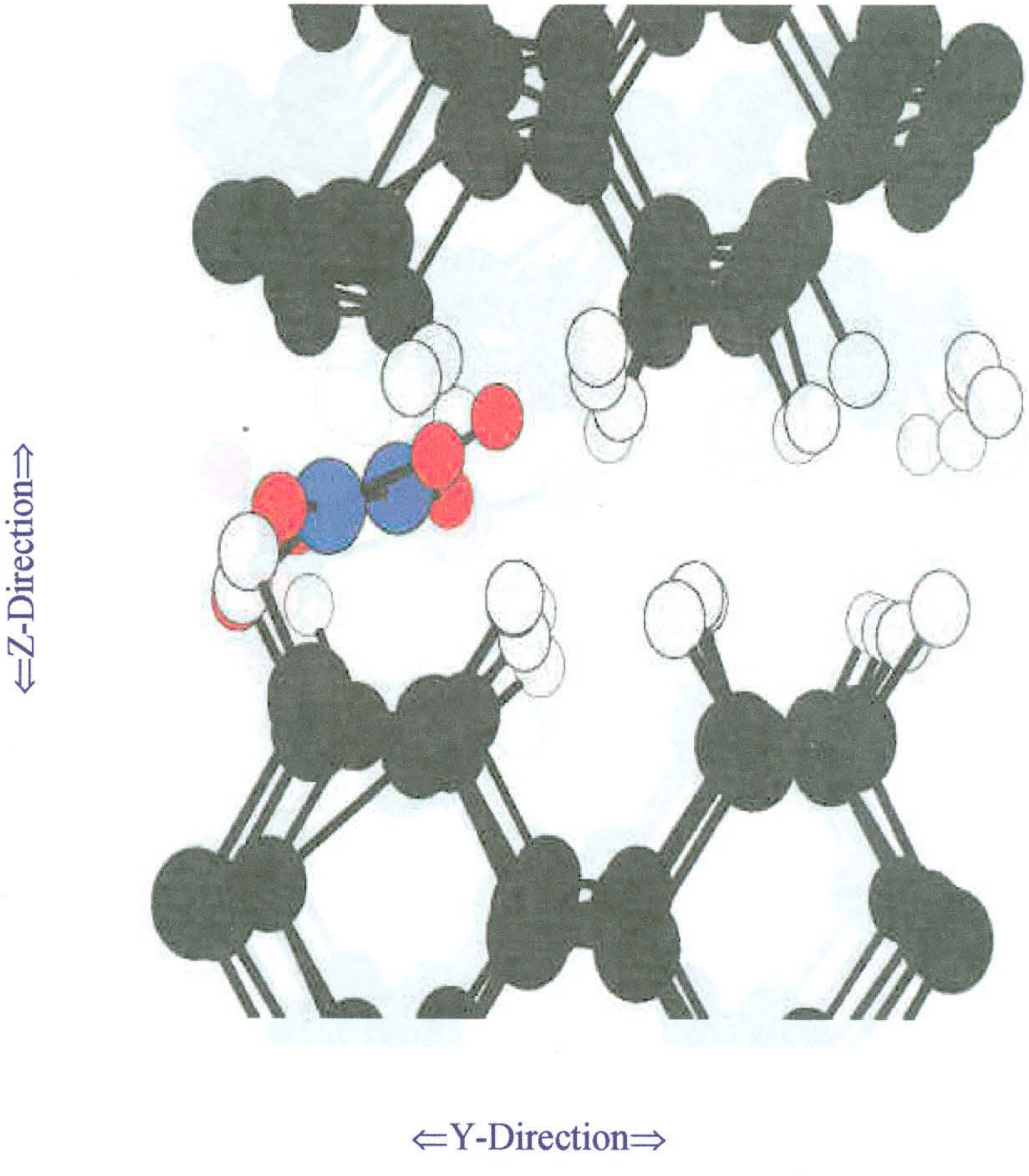


Figure 28

Ethane Molecule Between Surfaces

Ethane Movement - I-Trial Low Frictional Force

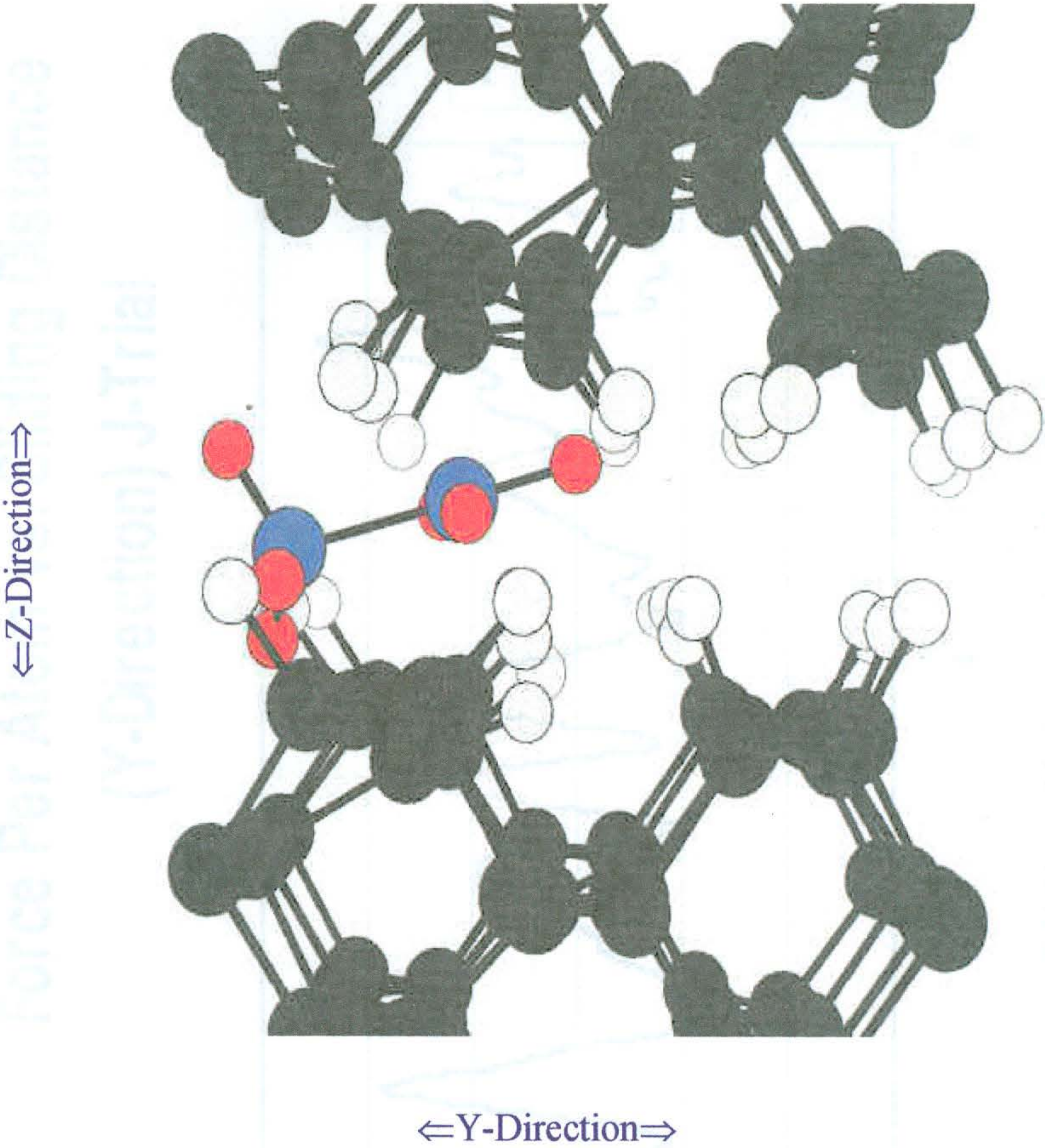


Figure 29

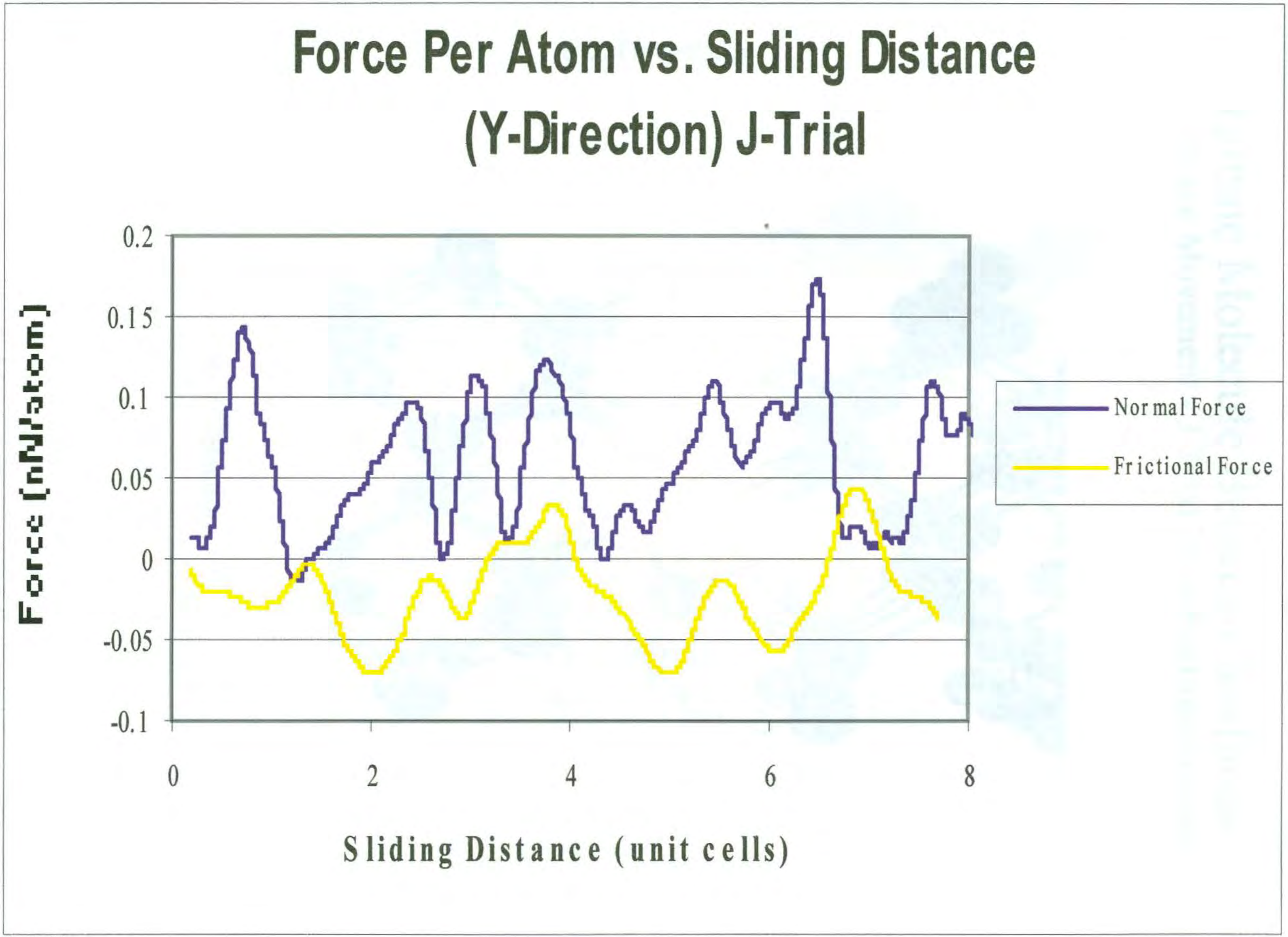

Force Per Atom vs. Sliding Distance (Y-Direction) J-Trial
Force (nN/atom)
0.2
0.15
0.1
0.05
0
-0.05
-0.1
0
2
4
6
8
Sliding Distance (unit cells)
Normal Force
Frictional Force

Figure 30

Ethane Molecule Between Surfaces

Ethane Movement - J-Trial High Frictional Force

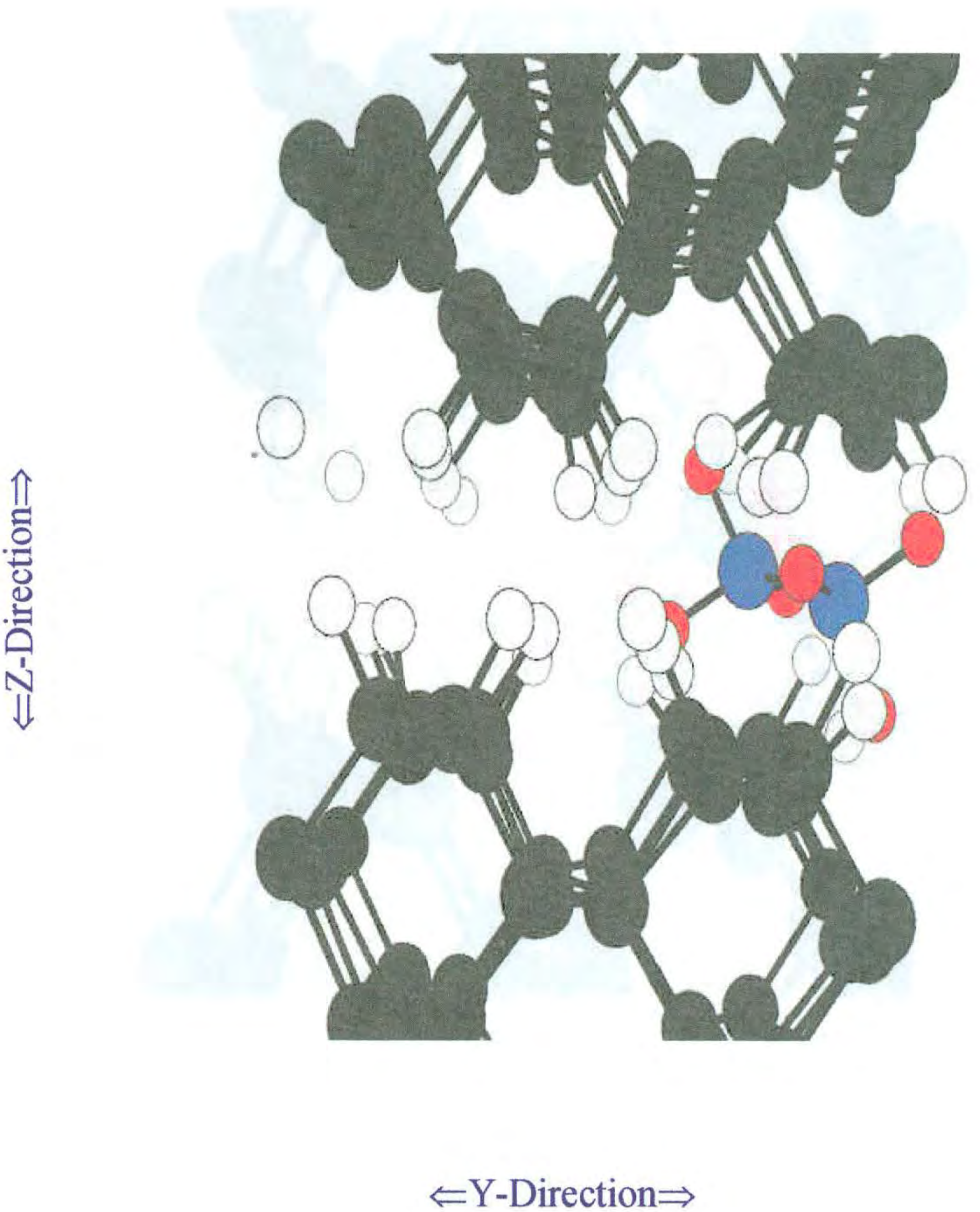


Figure 31

Ethane Molecule Between Surfaces

Ethane Movement - J-Trial Low Frictional Force

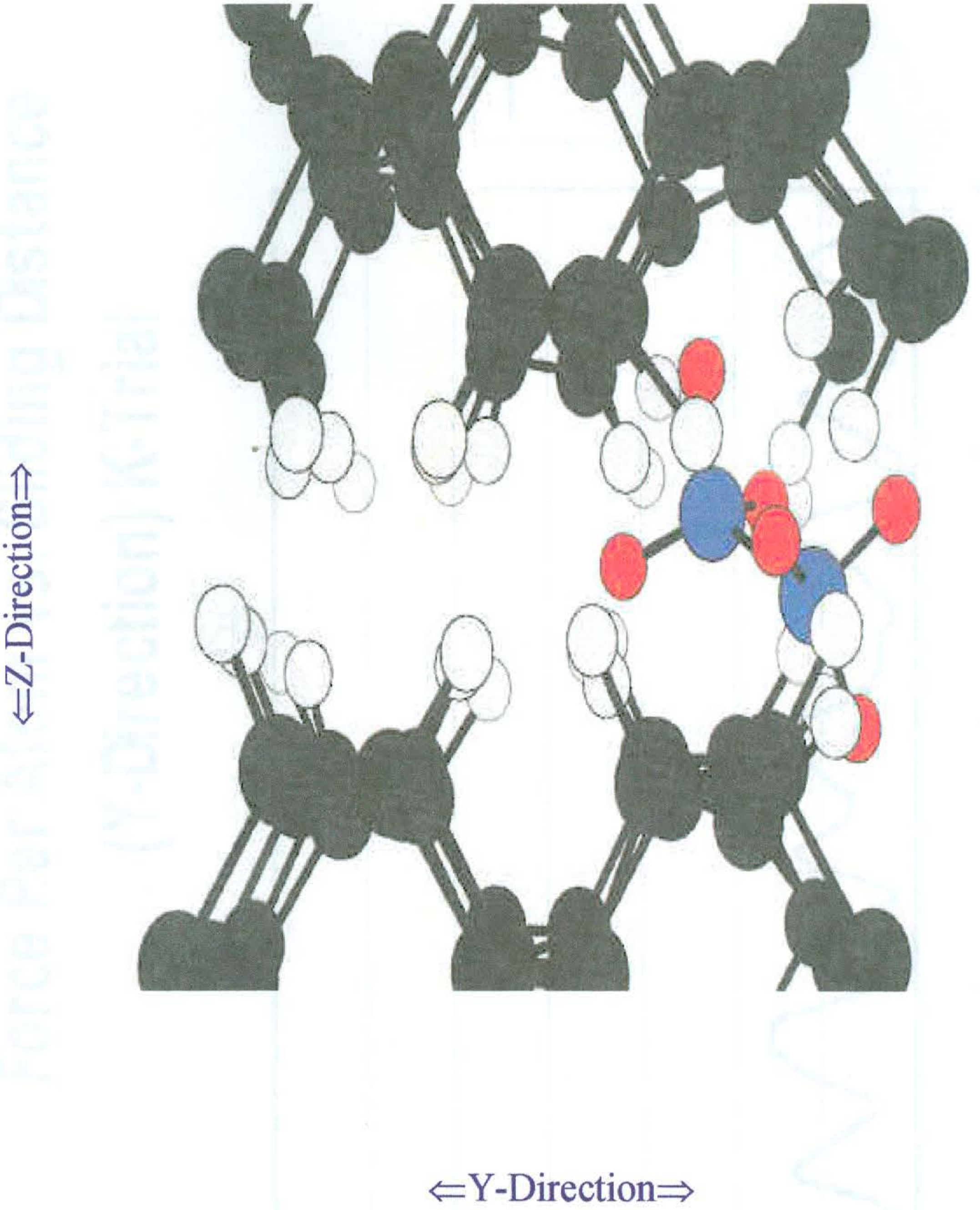


Figure 32

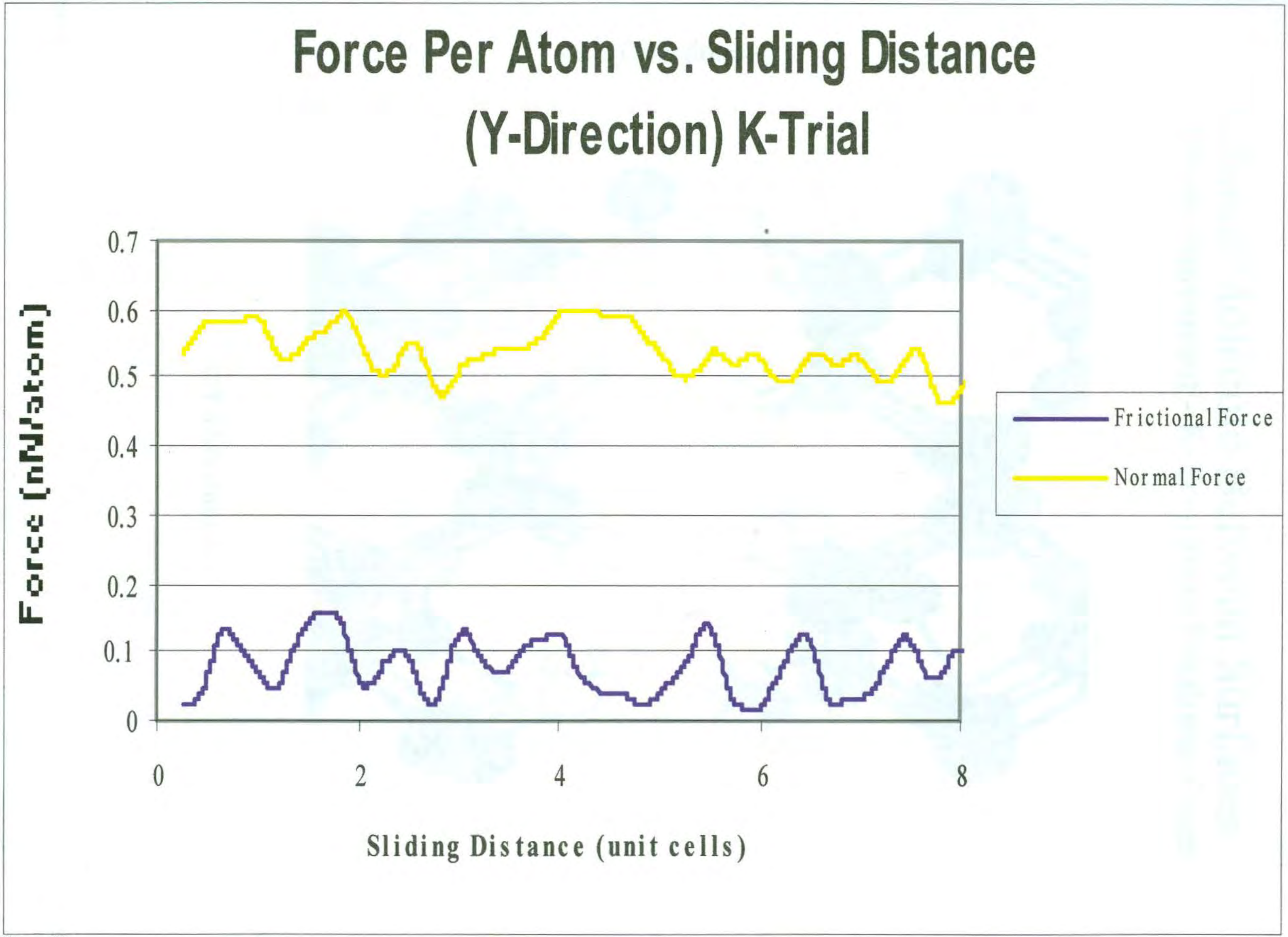
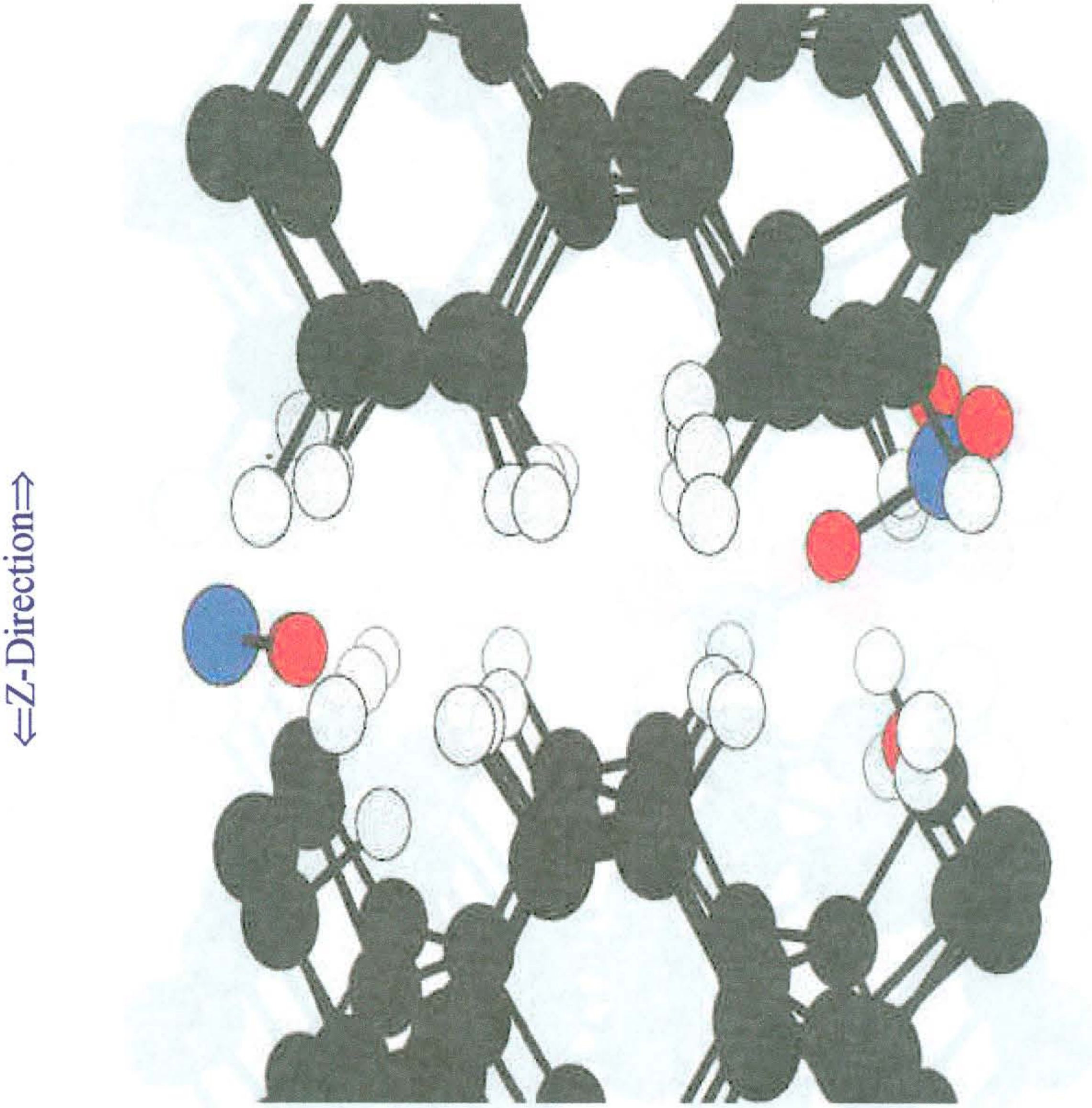

Force Per Atom vs. Sliding Distance (Y-Direction) K-Trial
Force (nN/atom)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 33

Ethane Molecule Between Surfaces

Ethane Movement - K-Trial High Frictional Force



⇐Y-Direction⇒

Figure 34

Ethane Molecule Between Surfaces

Ethane Movement - K-Trial Low Frictional Force

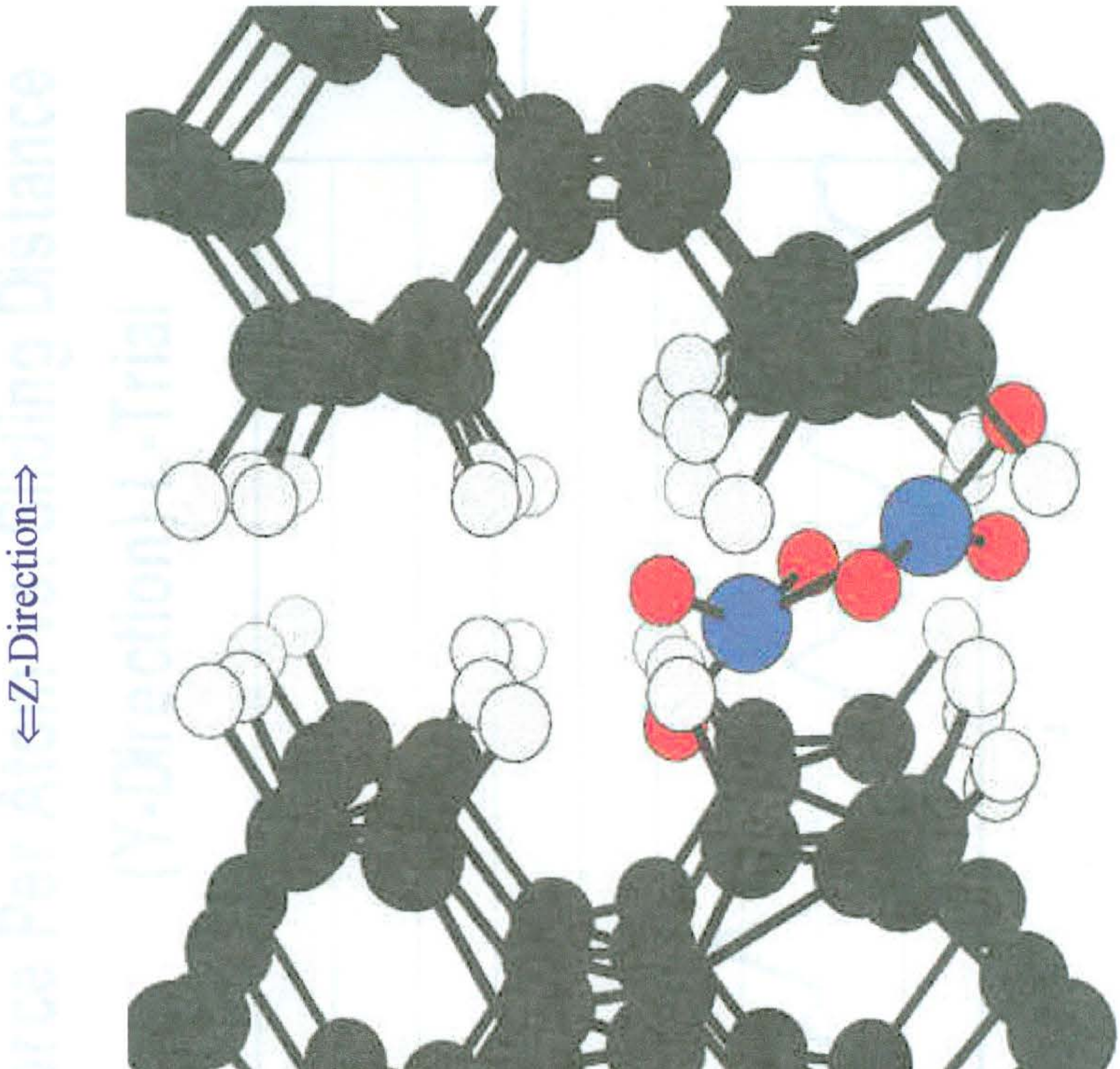


Figure 35

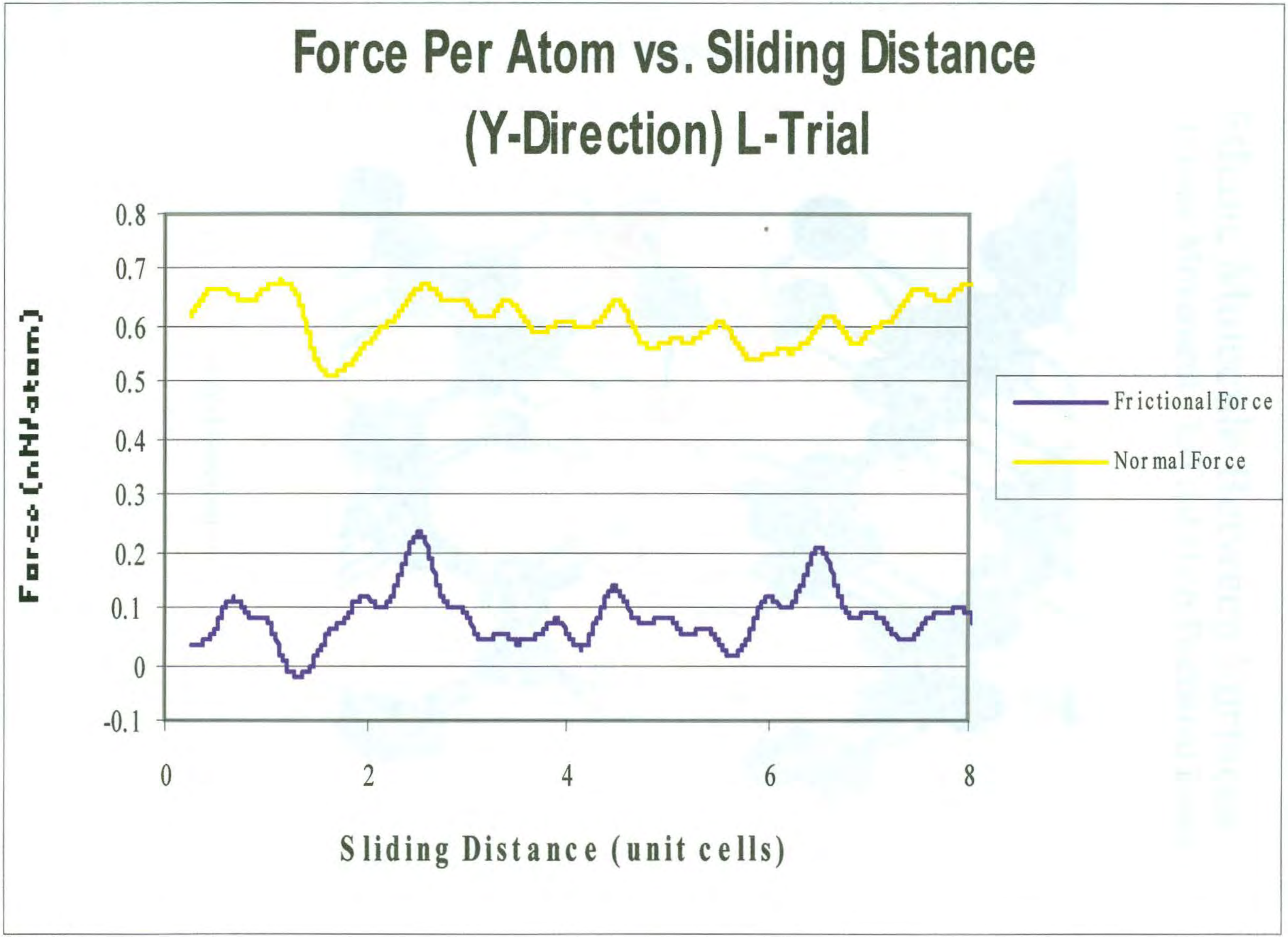

Force Per Atom vs. Sliding Distance (Y-Direction) L-Trial
Force (nN/atom)
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 36

Ethane Molecule Between Surfaces

Ethane Movement - L-Trial High Frictional Force

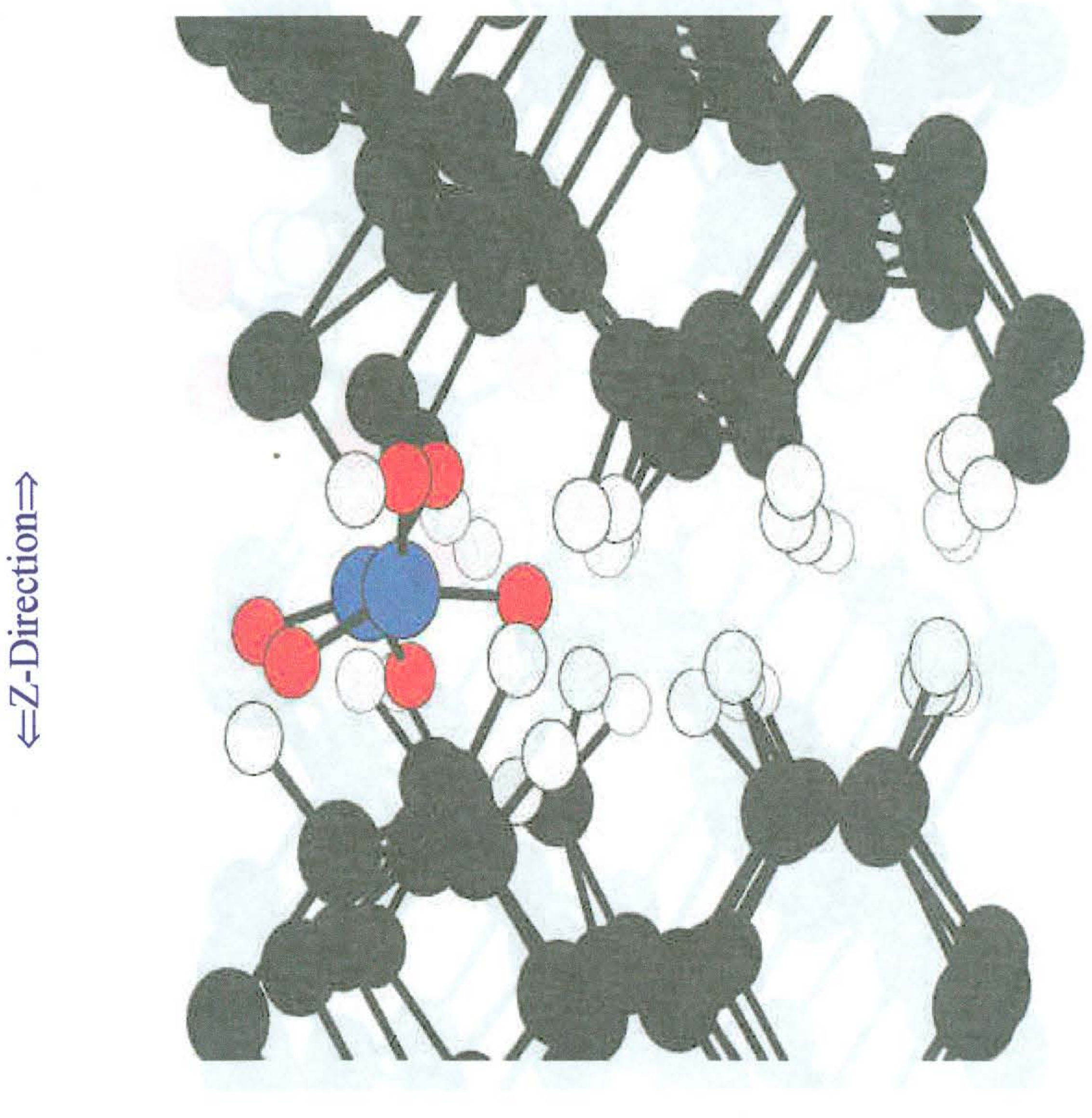


Figure 37

Ethane Molecule Between Surfaces

Ethane Movement - L-Trial Low Frictional Force

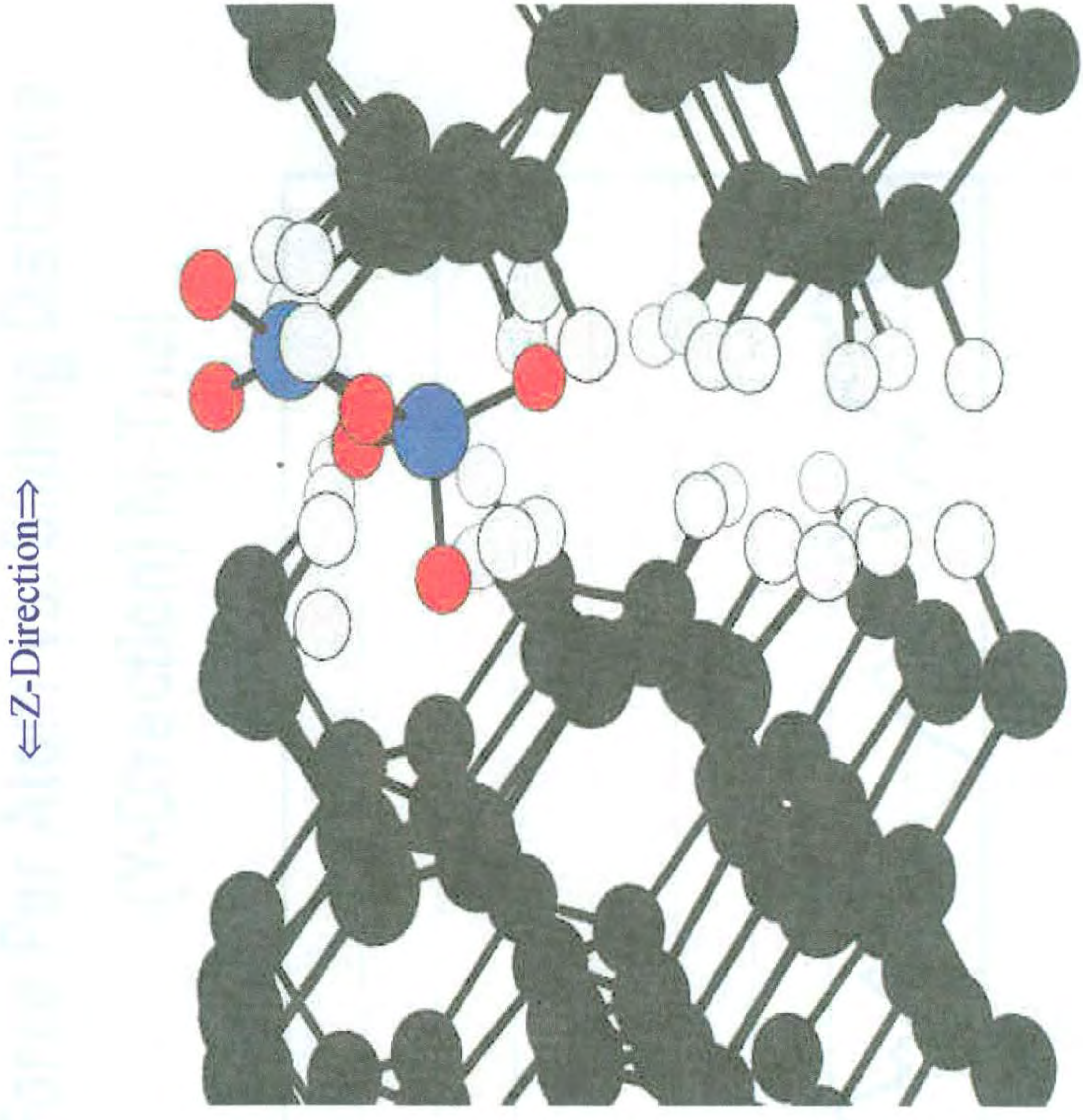


Figure 38

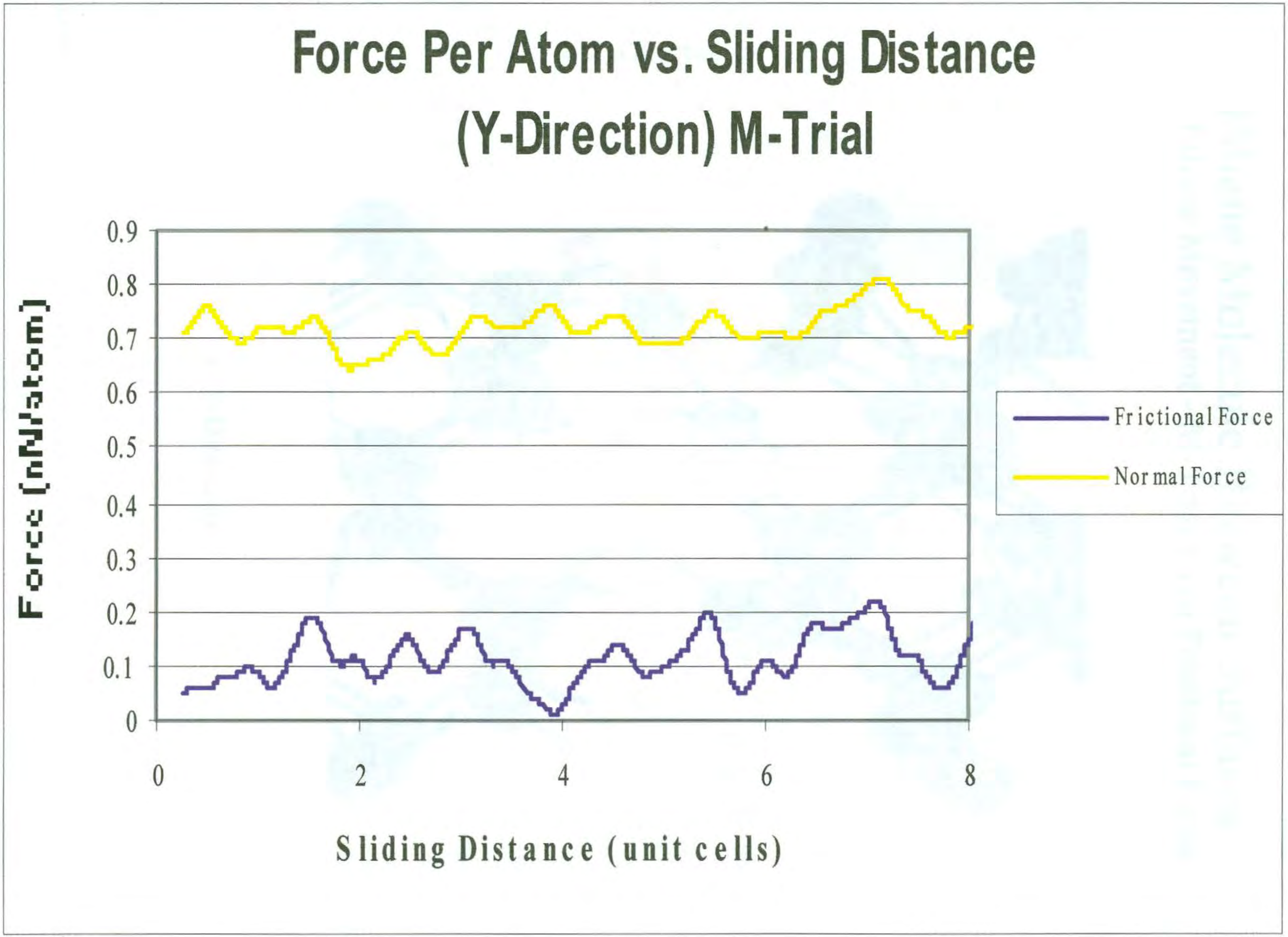
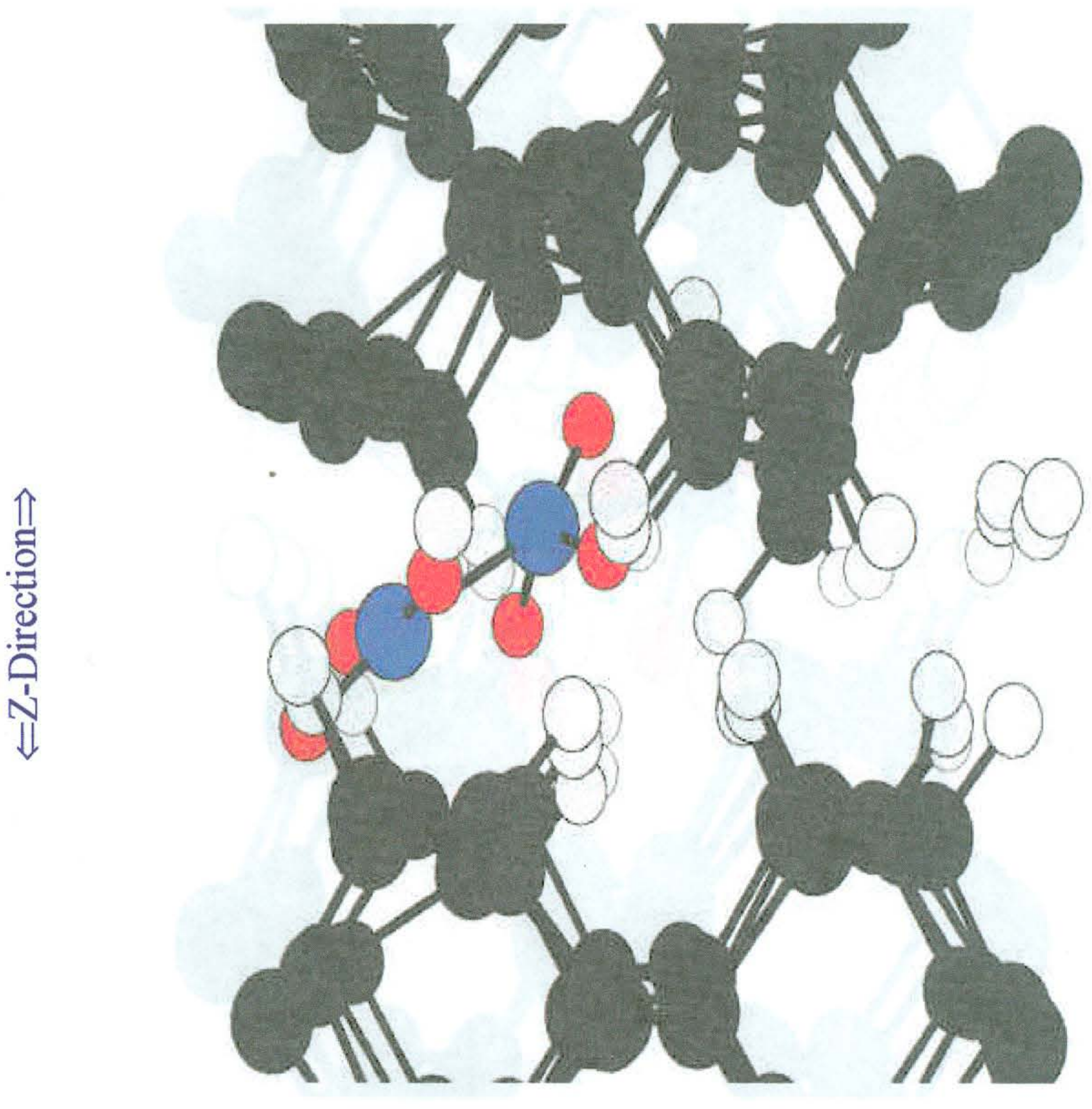

Force Per Atom vs. Sliding Distance (Y-Direction) M-Trial
Force (nN/atom)
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 39

Ethane Molecule Between Surfaces

Ethane Movement - M-Trial High Frictional Force



⇐Y-Direction⇒

Figure 40

Ethane Molecule Between Surfaces

Ethane Movement - M-Trial Low Frictional Force

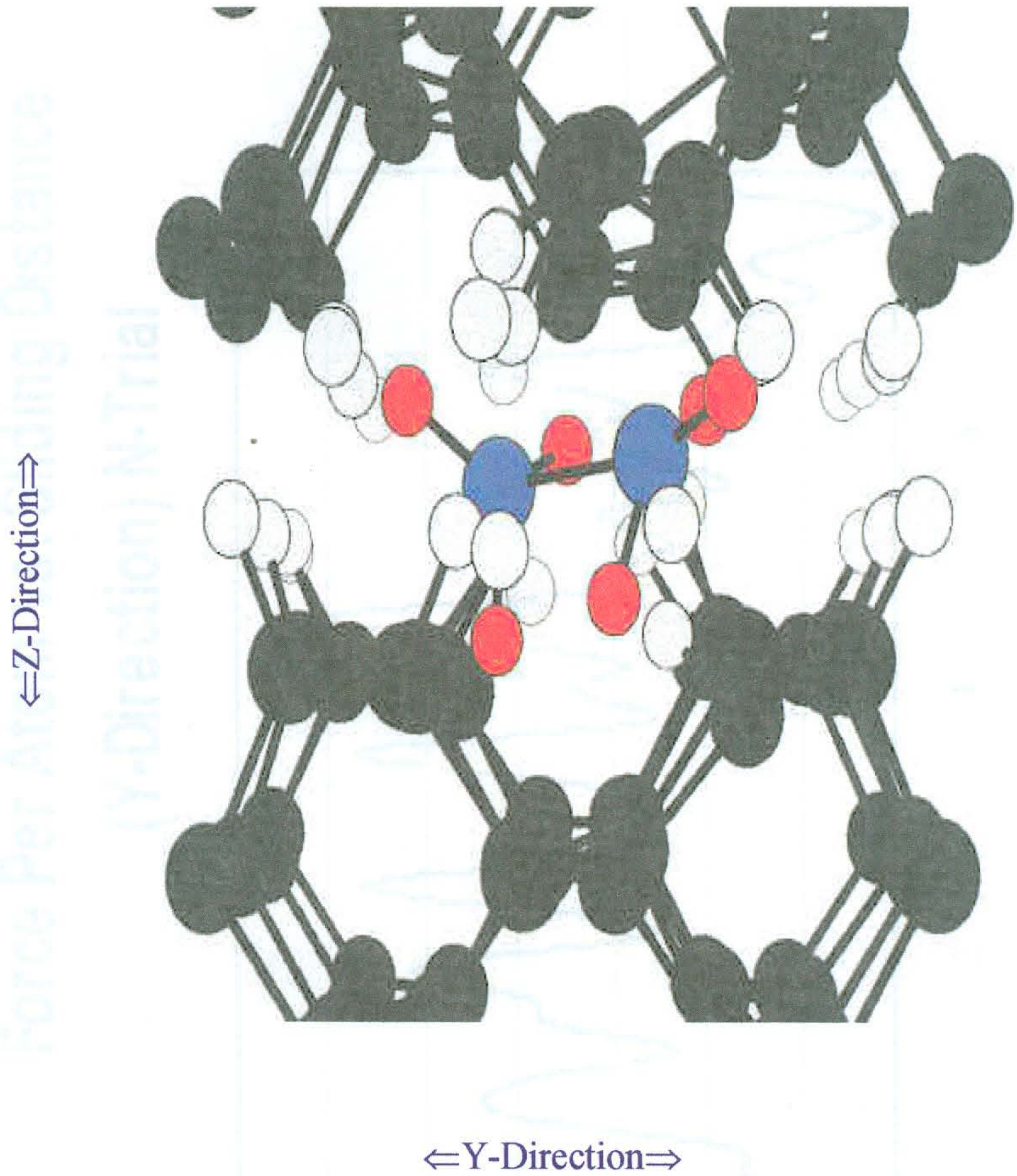


Figure 41

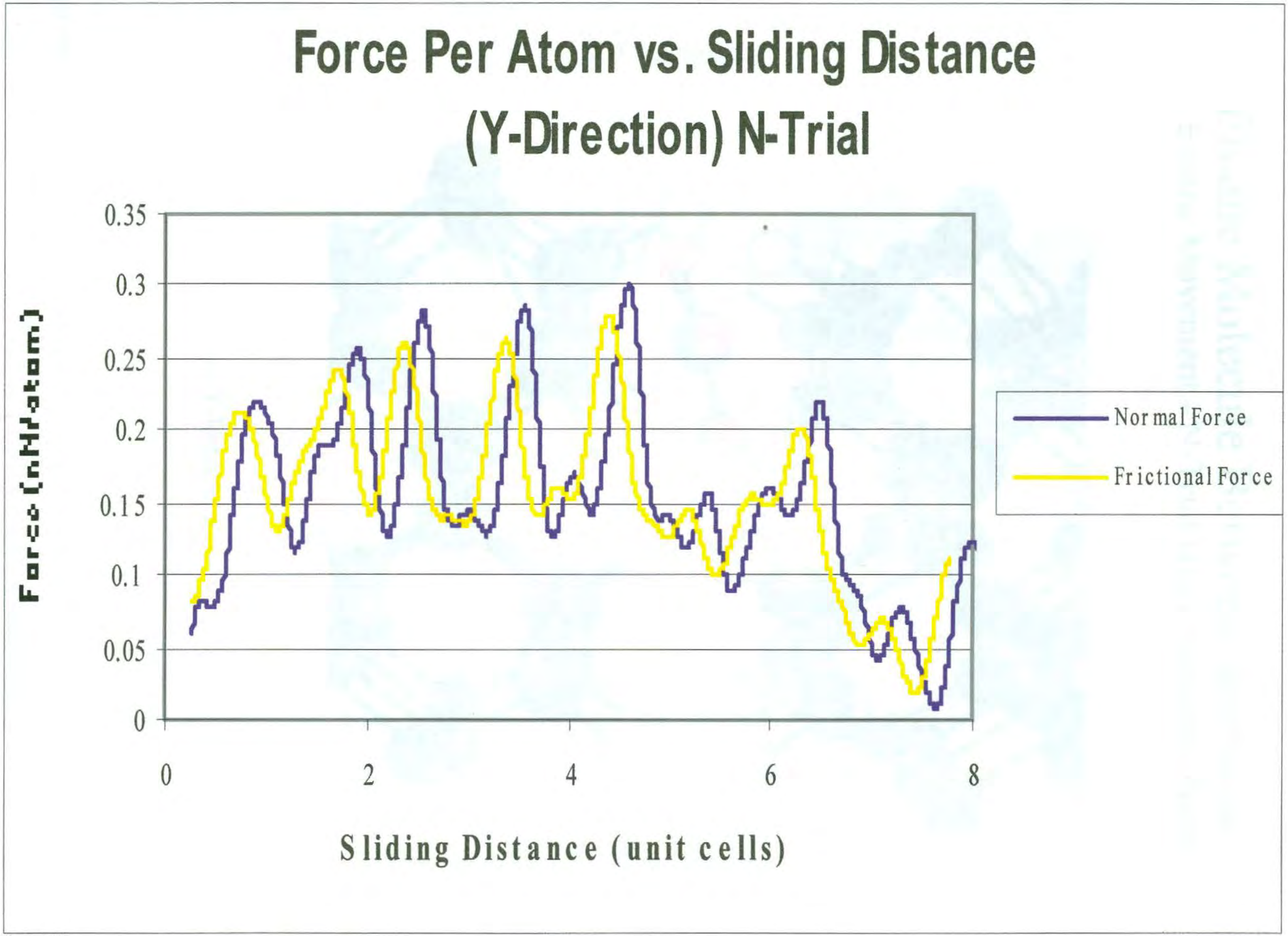

Force Per Atom vs. Sliding Distance (Y-Direction) N-Trial
Force (nN/atom)
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
2
4
6
8
Sliding Distance (unit cells)
Normal Force
Frictional Force

Figure 42

Ethane Molecule Between Surfaces

Ethane Movement - N-Trial High Frictional Force

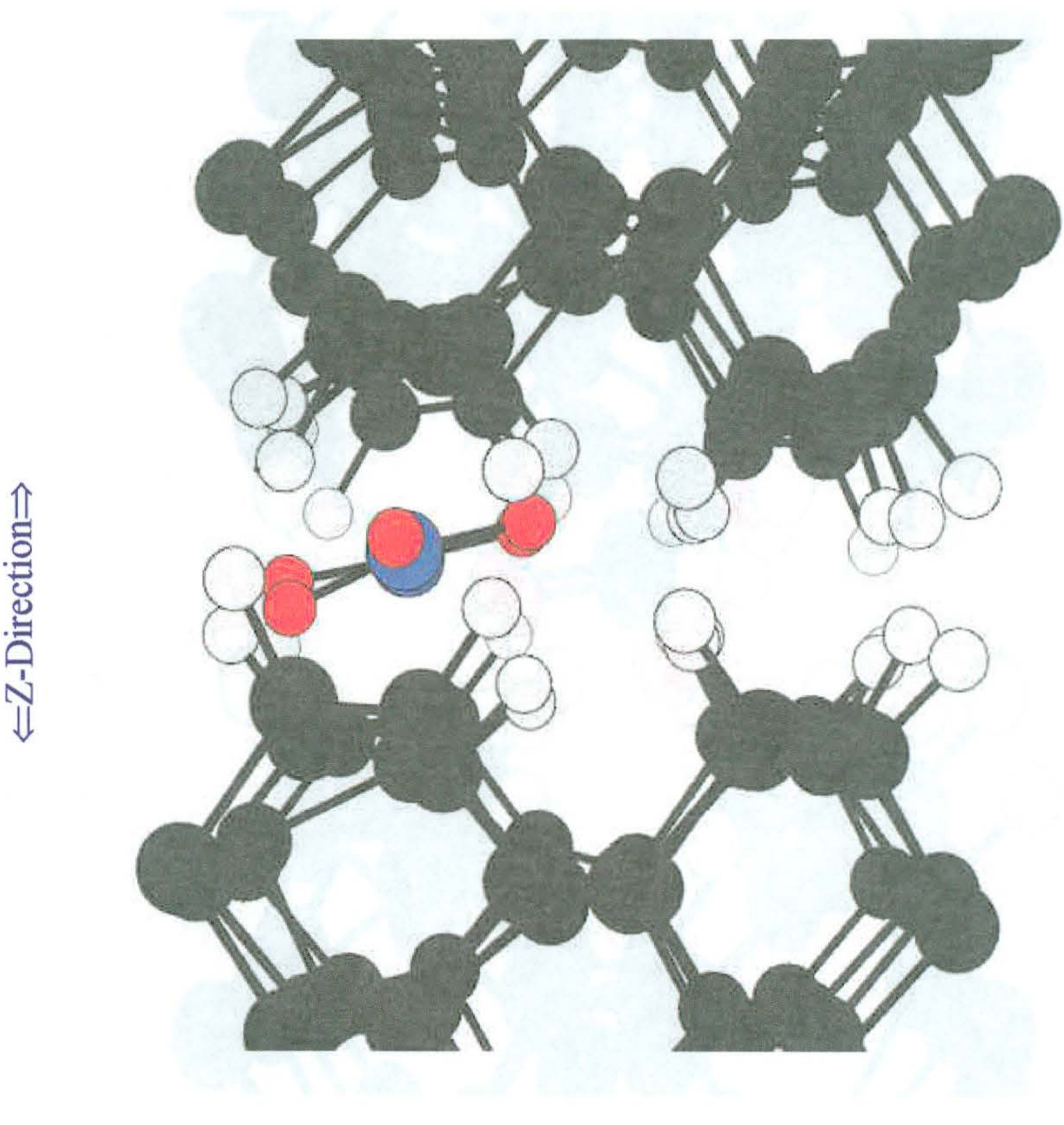


Figure 43

Ethane Molecule Between Surfaces

Ethane Movement - N-Trial Low Frictional Force

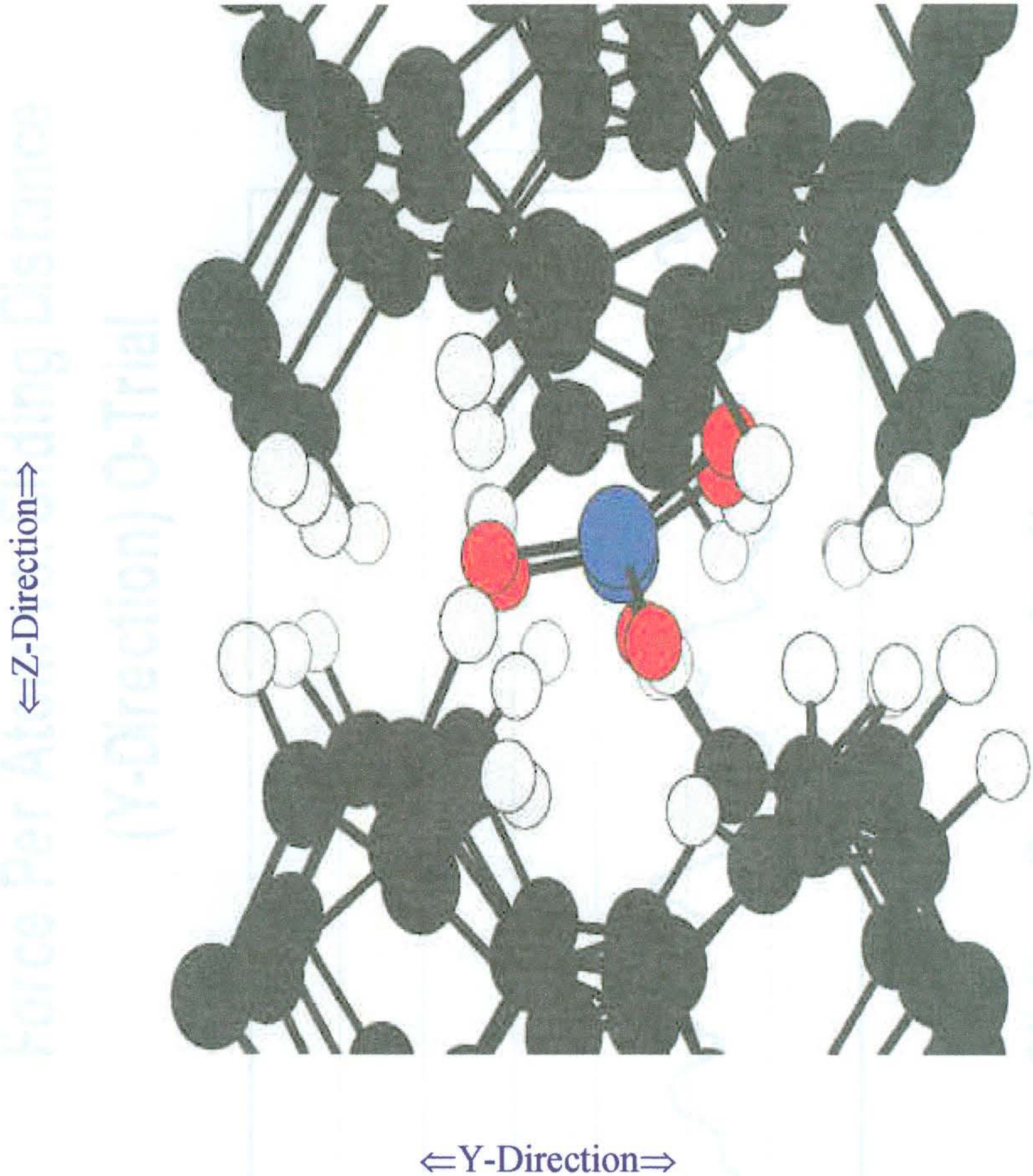


Figure 44

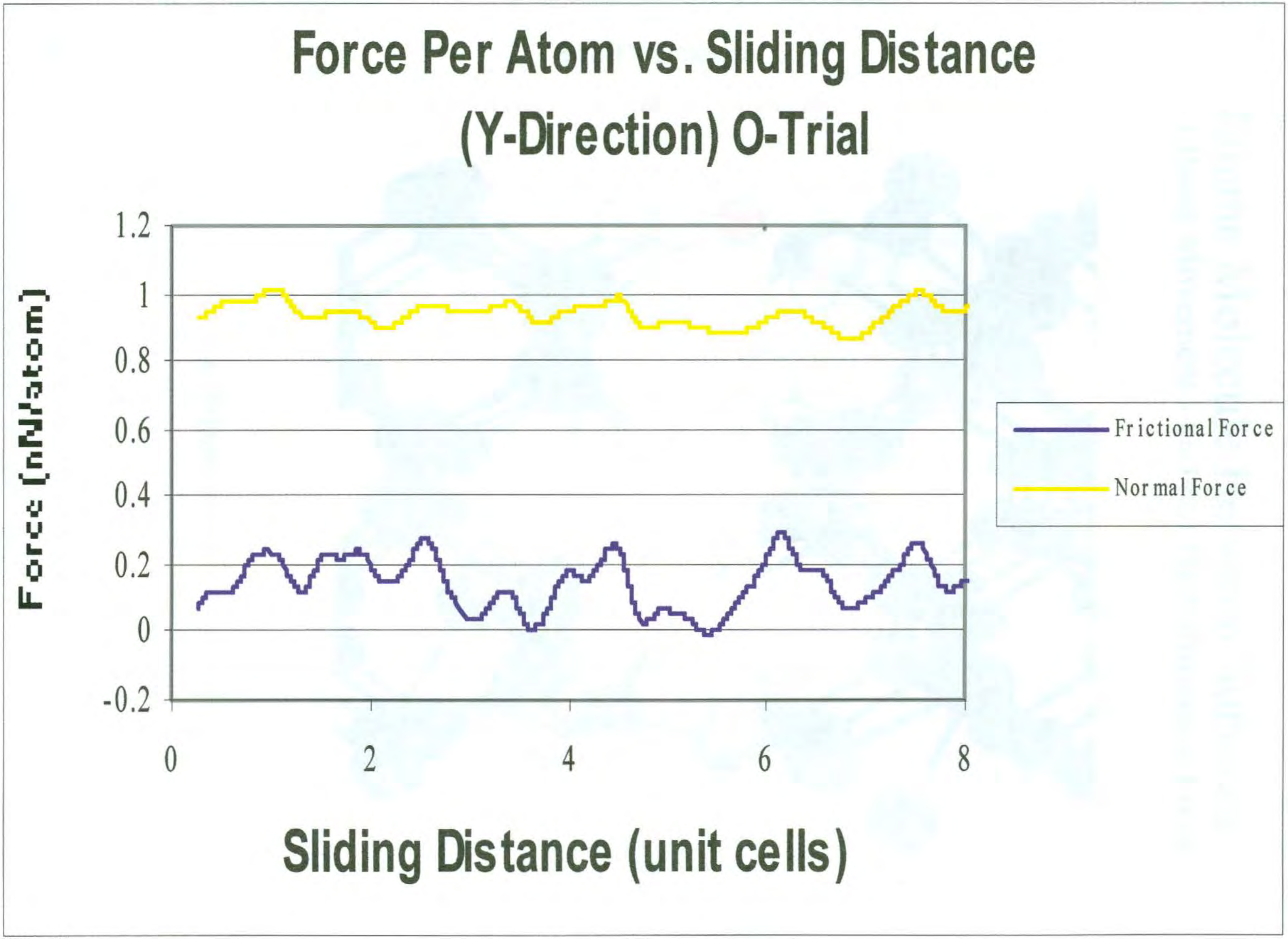

Force Per Atom vs. Sliding Distance (Y-Direction) O-Trial
Force (nN/atom)
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 45

Ethane Molecule Between Surfaces
Ethane Movement - O-Trial High Frictional Force

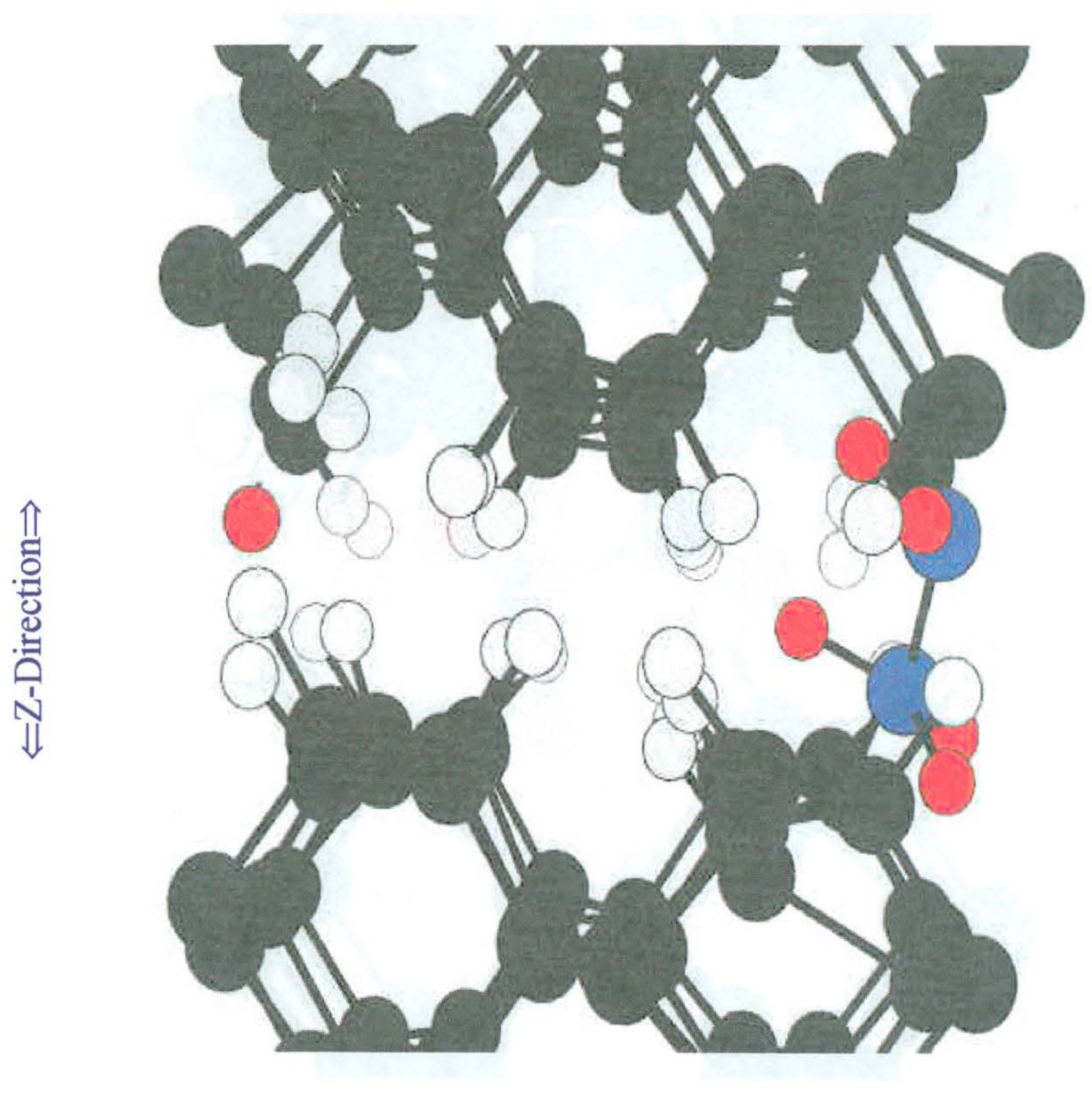


Figure 46

Ethane Molecule Between Surfaces

Ethane Movement - O-Trial Low Frictional Force

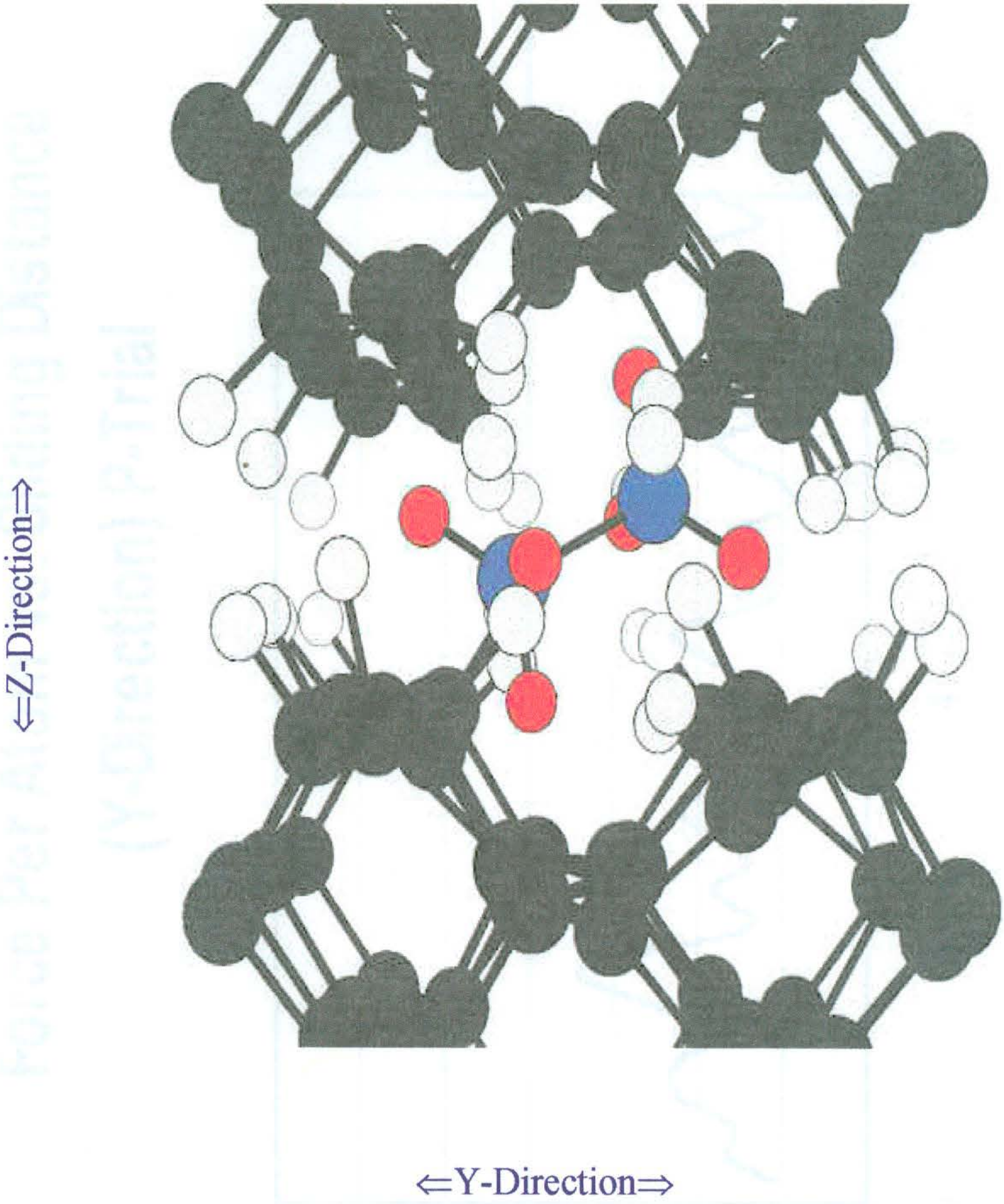
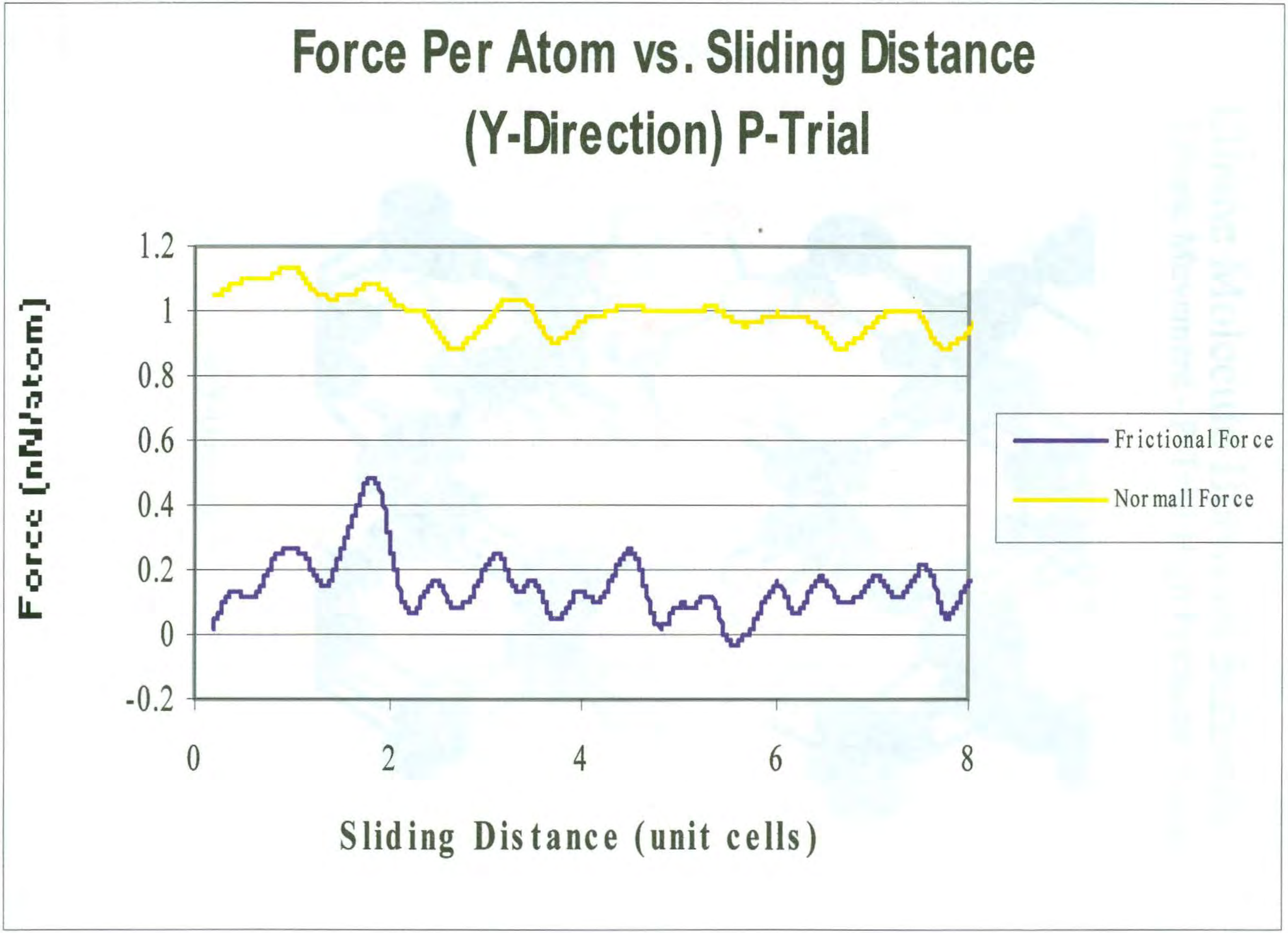


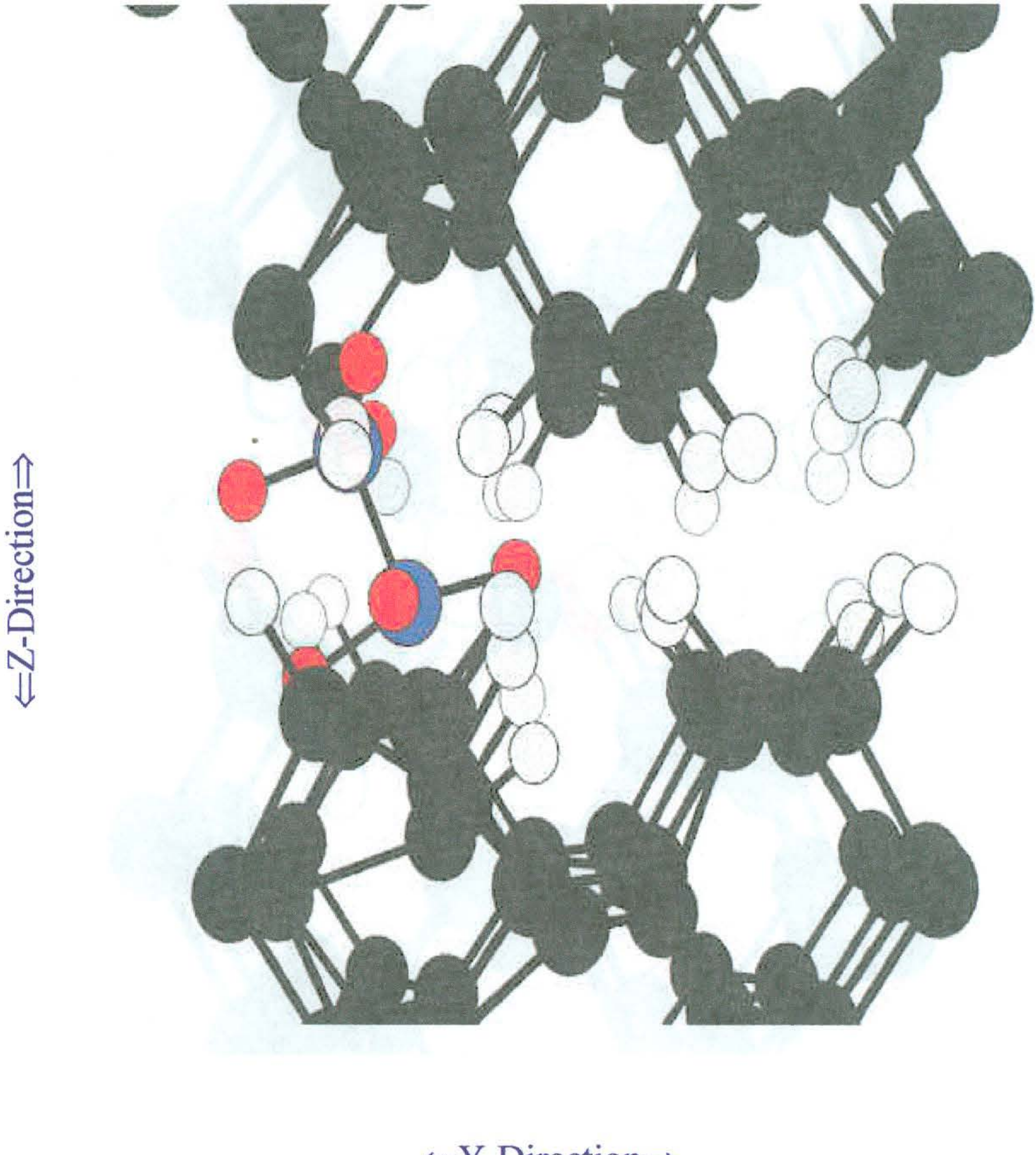
Figure 47



Force Per Atom vs. Sliding Distance (Y-Direction) P-Trial

Ethane Molecule Between Surfaces

Ethane Movement - P-Trial High Frictional Force



⇐Y-Direction⇒

Figure 49

Ethane Molecule Between Surfaces

Ethane Movement - P-Trial Low Frictional Force

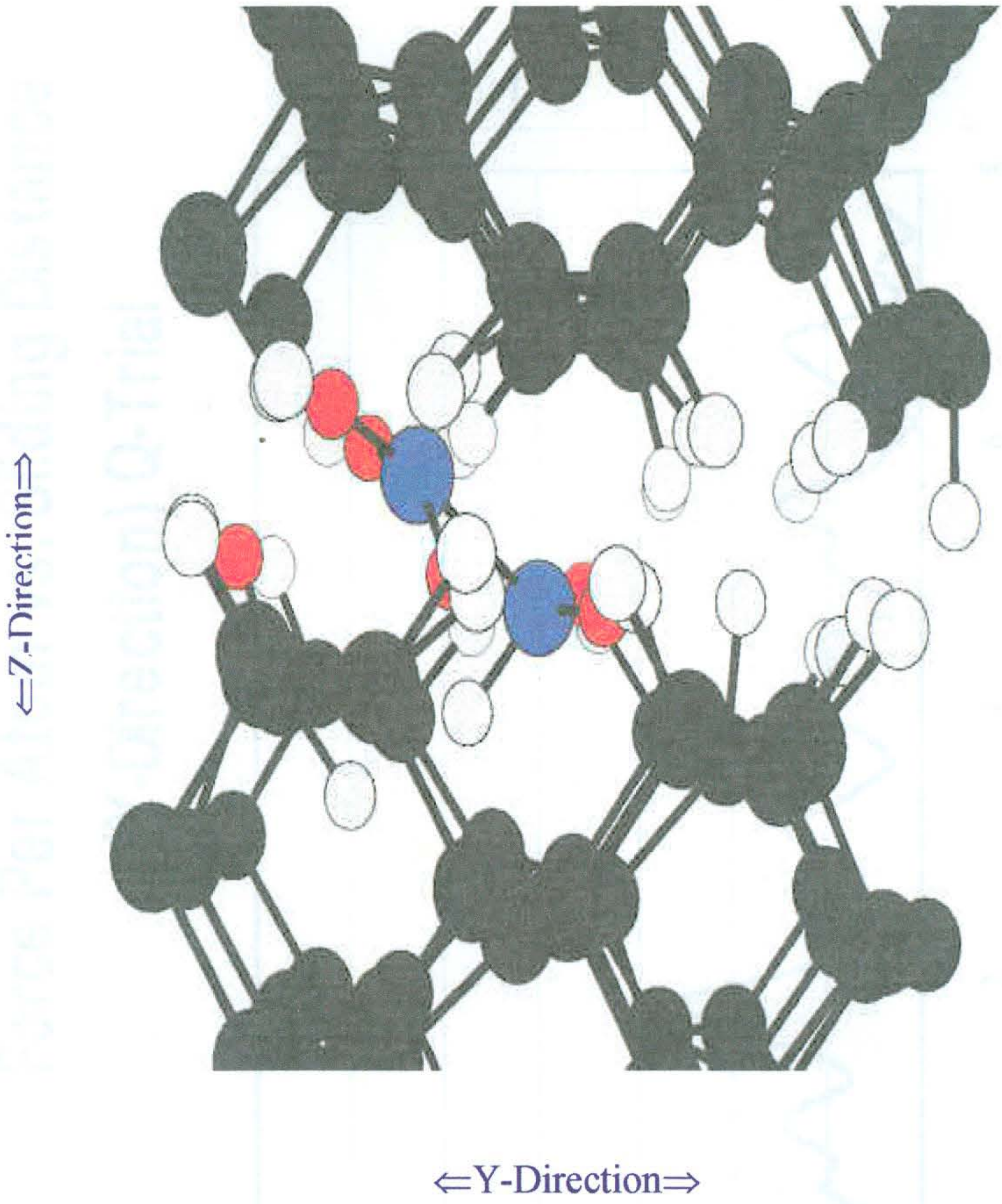


Figure 50

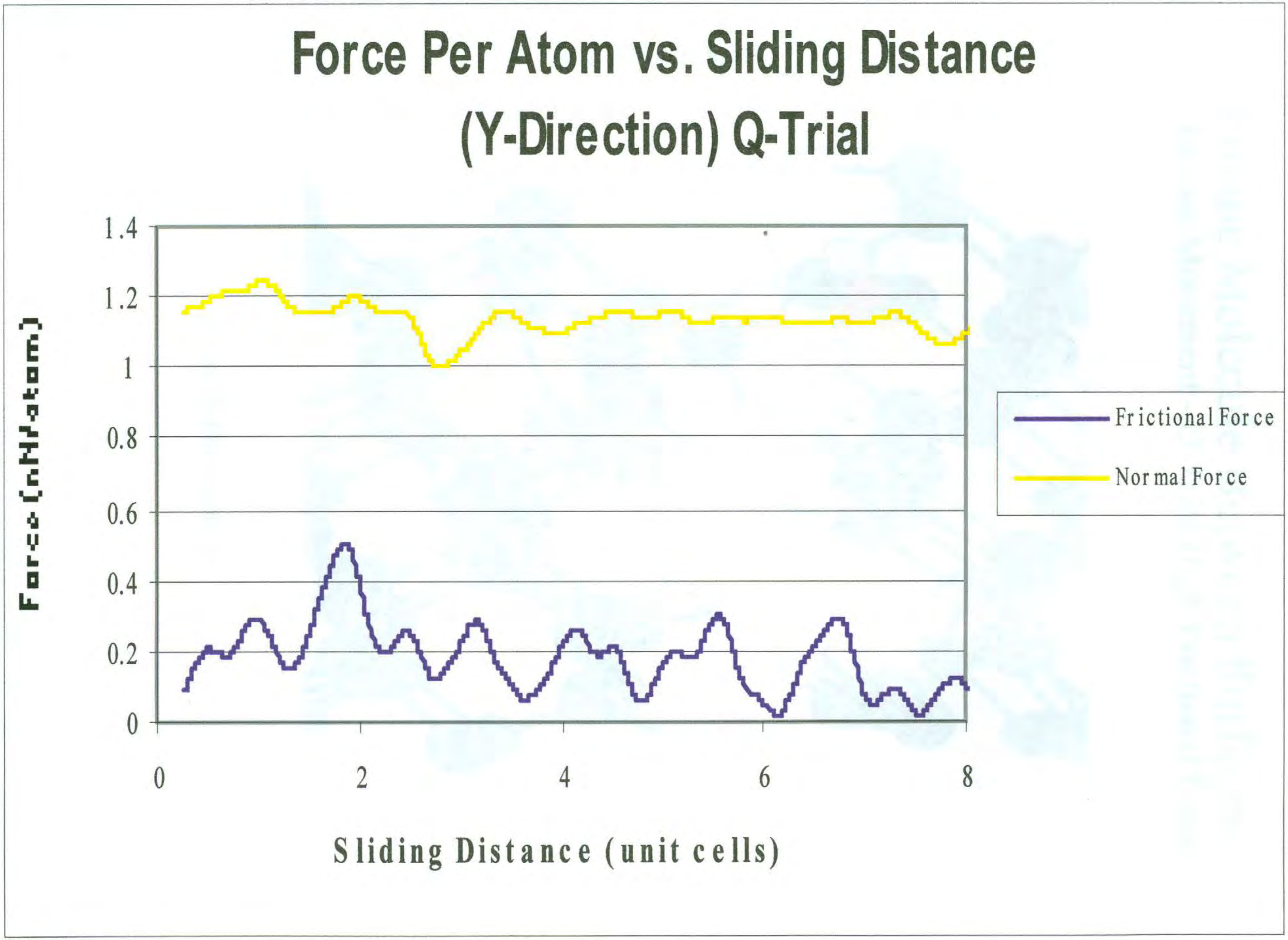

Force Per Atom vs. Sliding Distance
(Y-Direction) Q-Trial
Force (nN/atom)
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
2
4
6
8
Sliding Distance (unit cells)
Frictional Force
Normal Force

Figure 51

Ethane Molecule Between Surfaces

Ethane Movement - Q-Trial High Frictional Force

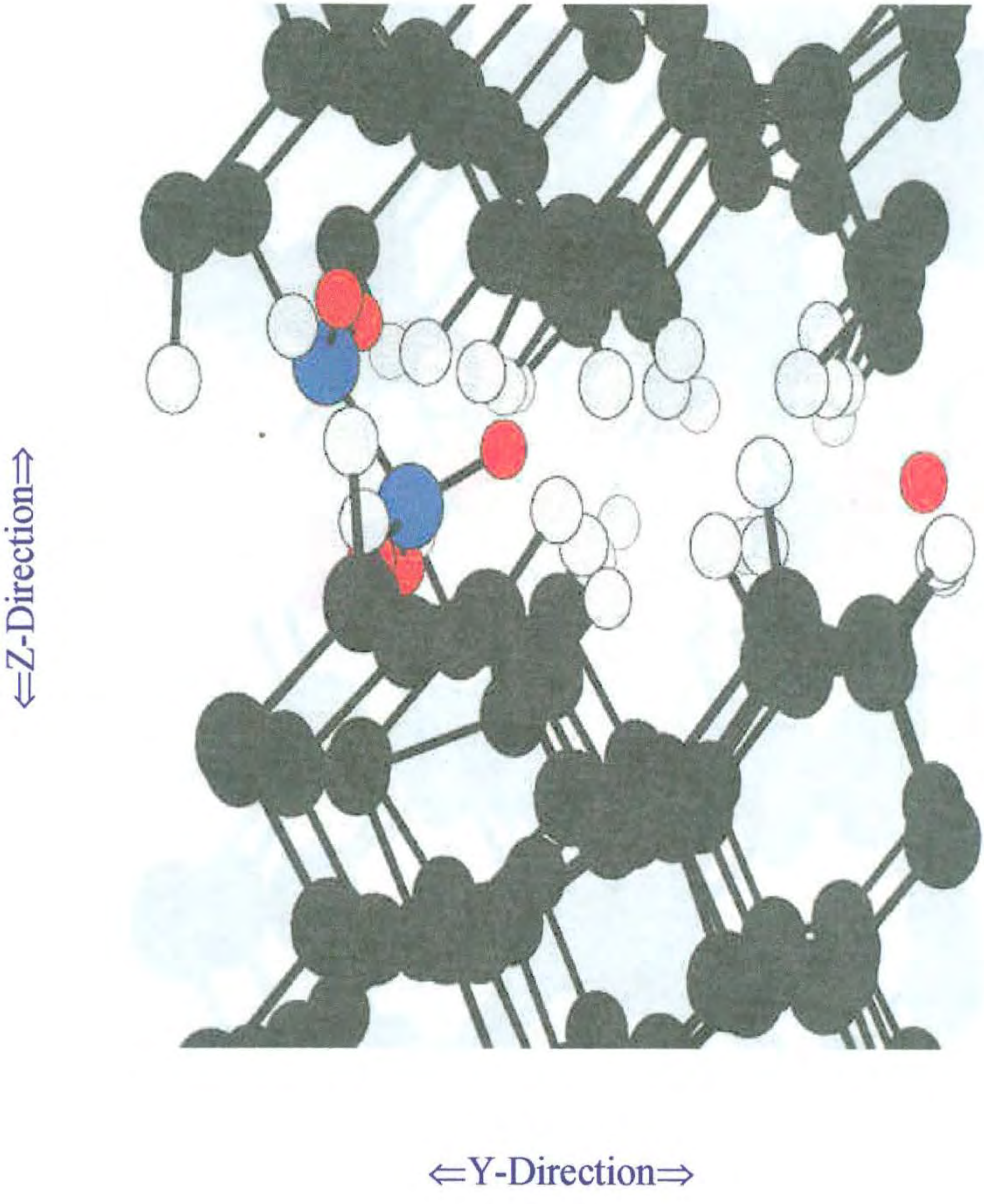


Figure 52

Ethane Molecule Between Surfaces

Ethane Movement - Q-Trial Low Frictional Force

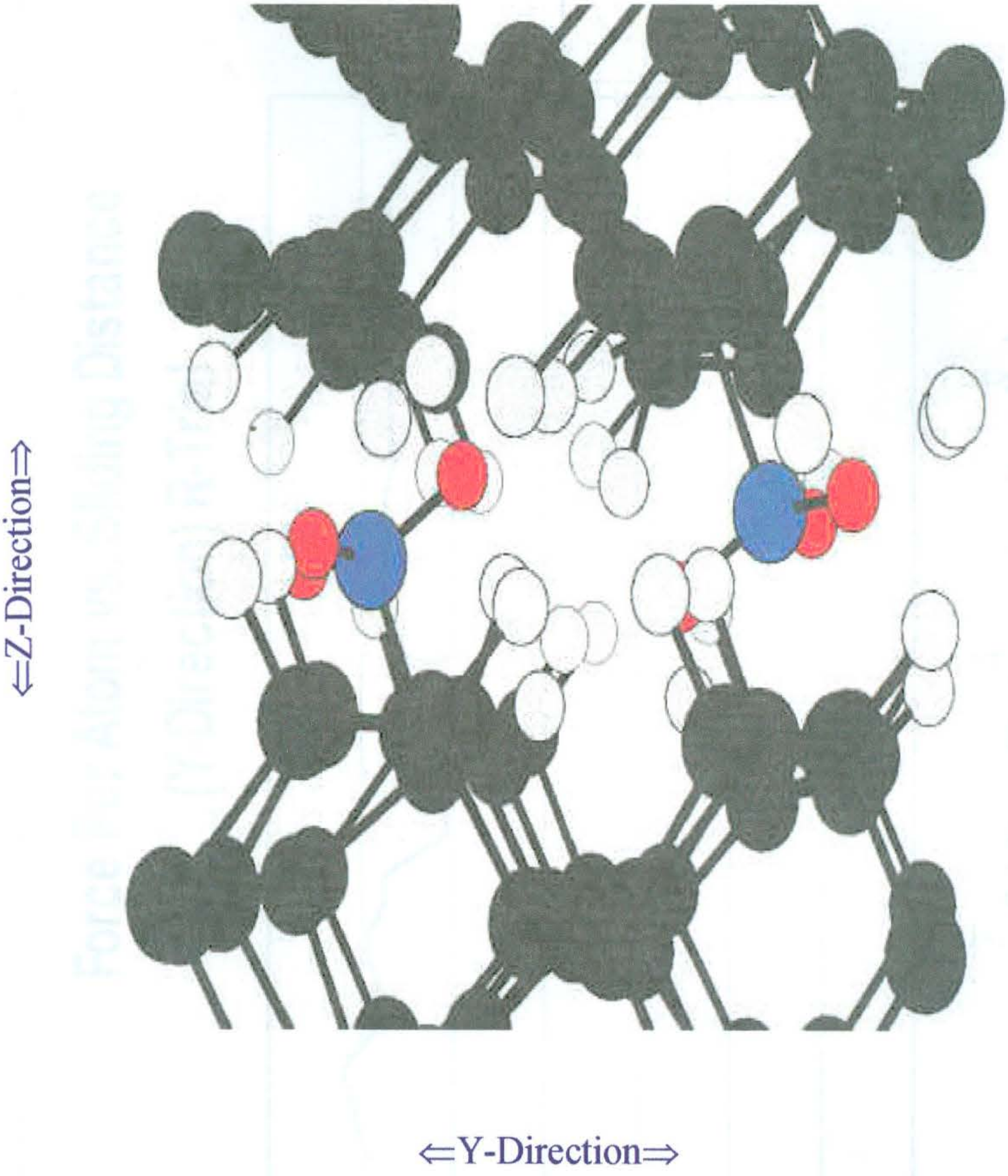


Figure 53

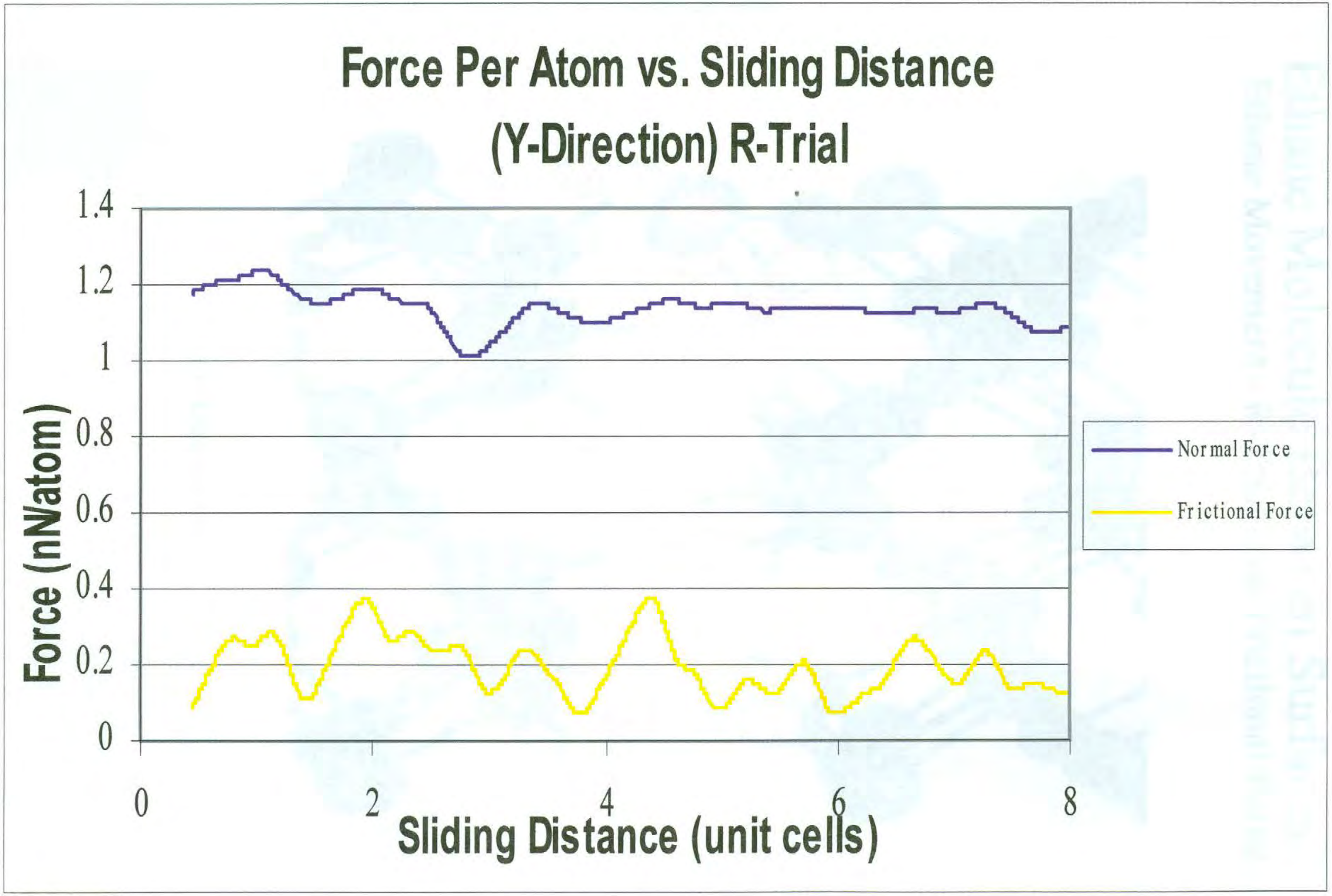

Force Per Atom vs. Sliding Distance (Y-Direction) R-Trial
Force (nN/atom)
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
2
4
6
8
Sliding Distance (unit cells)
Normal Force
Frictional Force

Figure 54

Ethane Molecule Between Surfaces

Ethane Movement - R-Trial Low Frictional Force

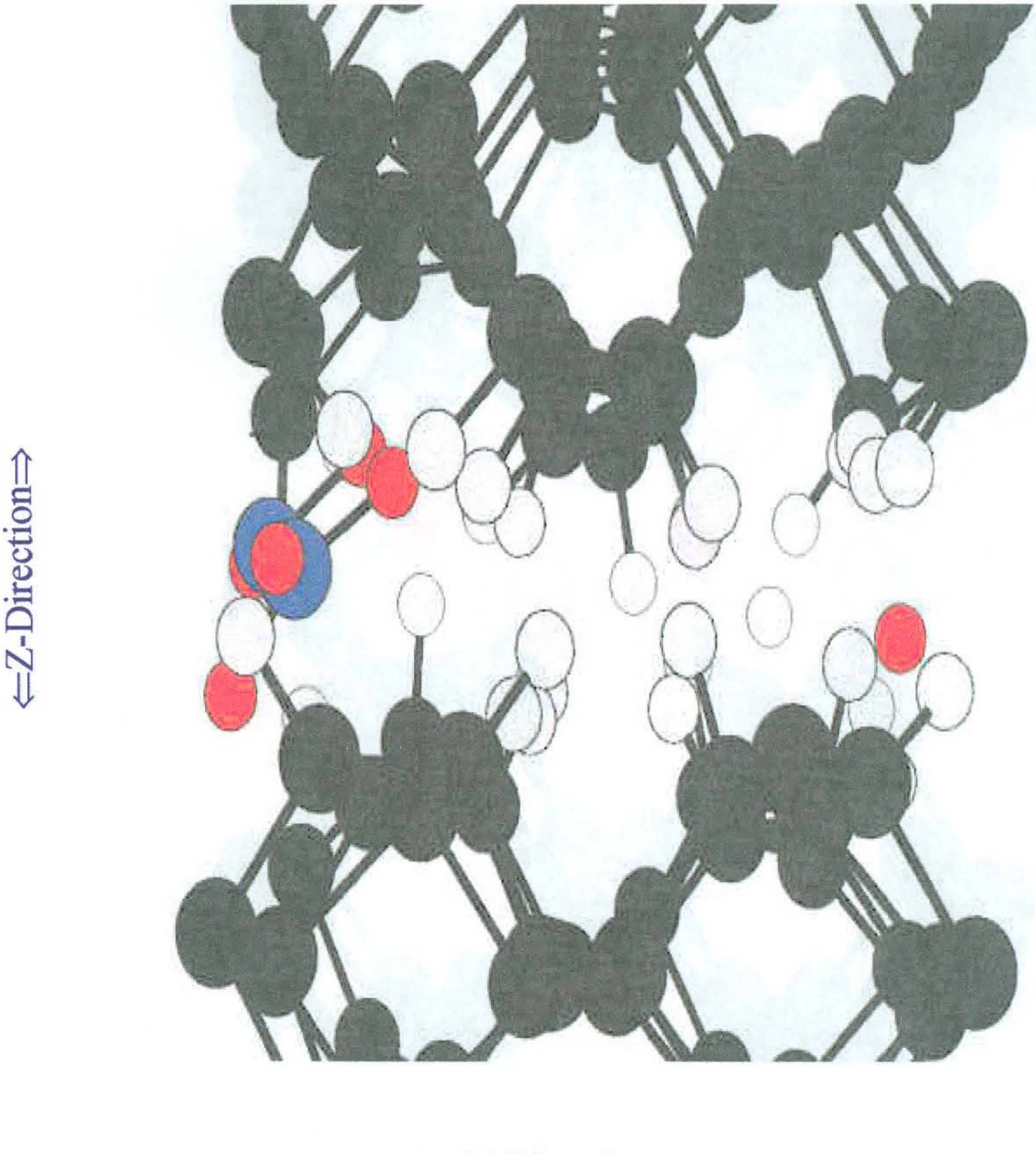


Figure 55

Ethane Molecule Between Surfaces

Ethane Movement - R-Trial Flat Frictional Force

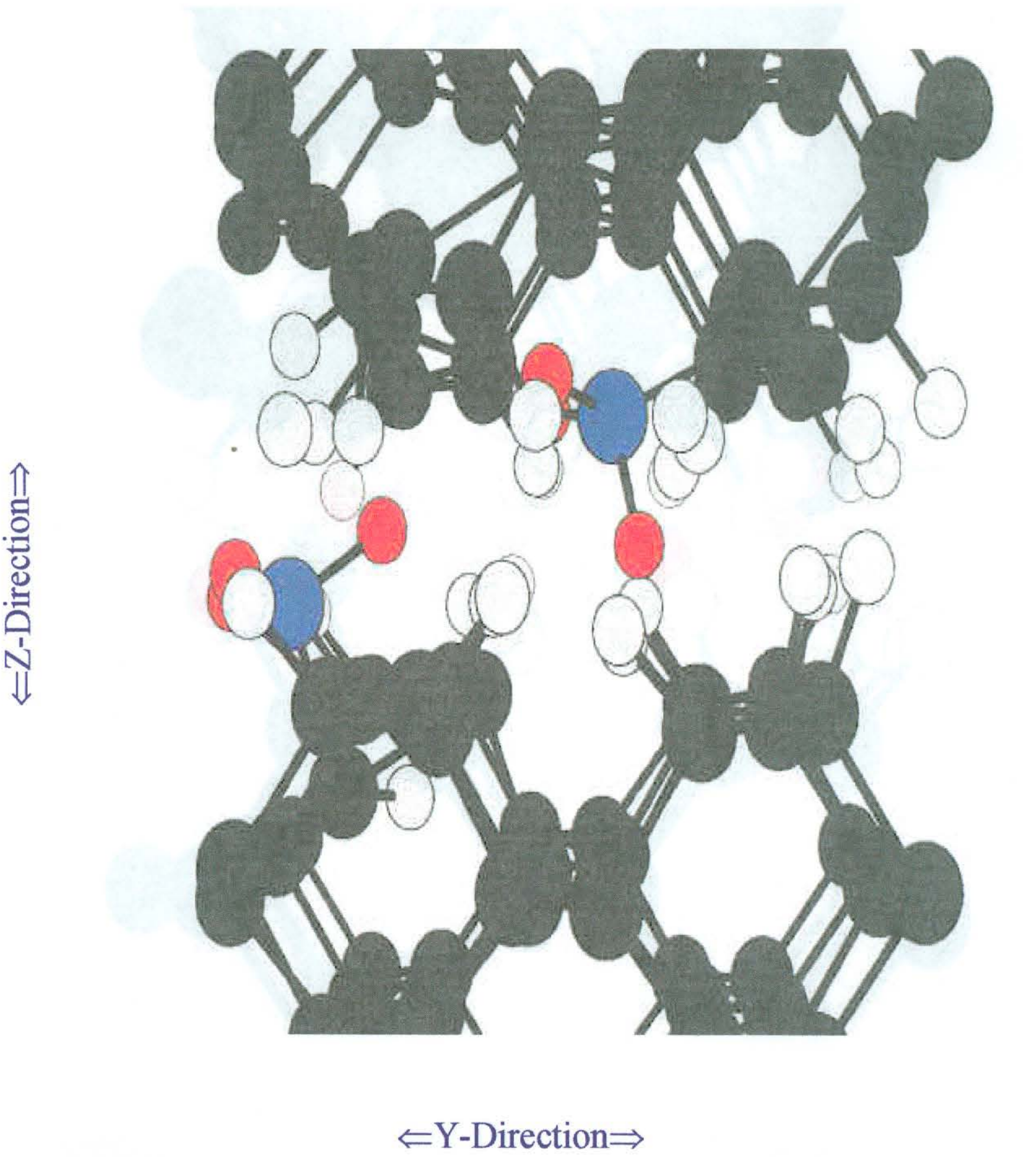


Figure 56

Ethane Molecule Between Surfaces

Ethane Movement - R-Trial 2nd Low Frictional Force

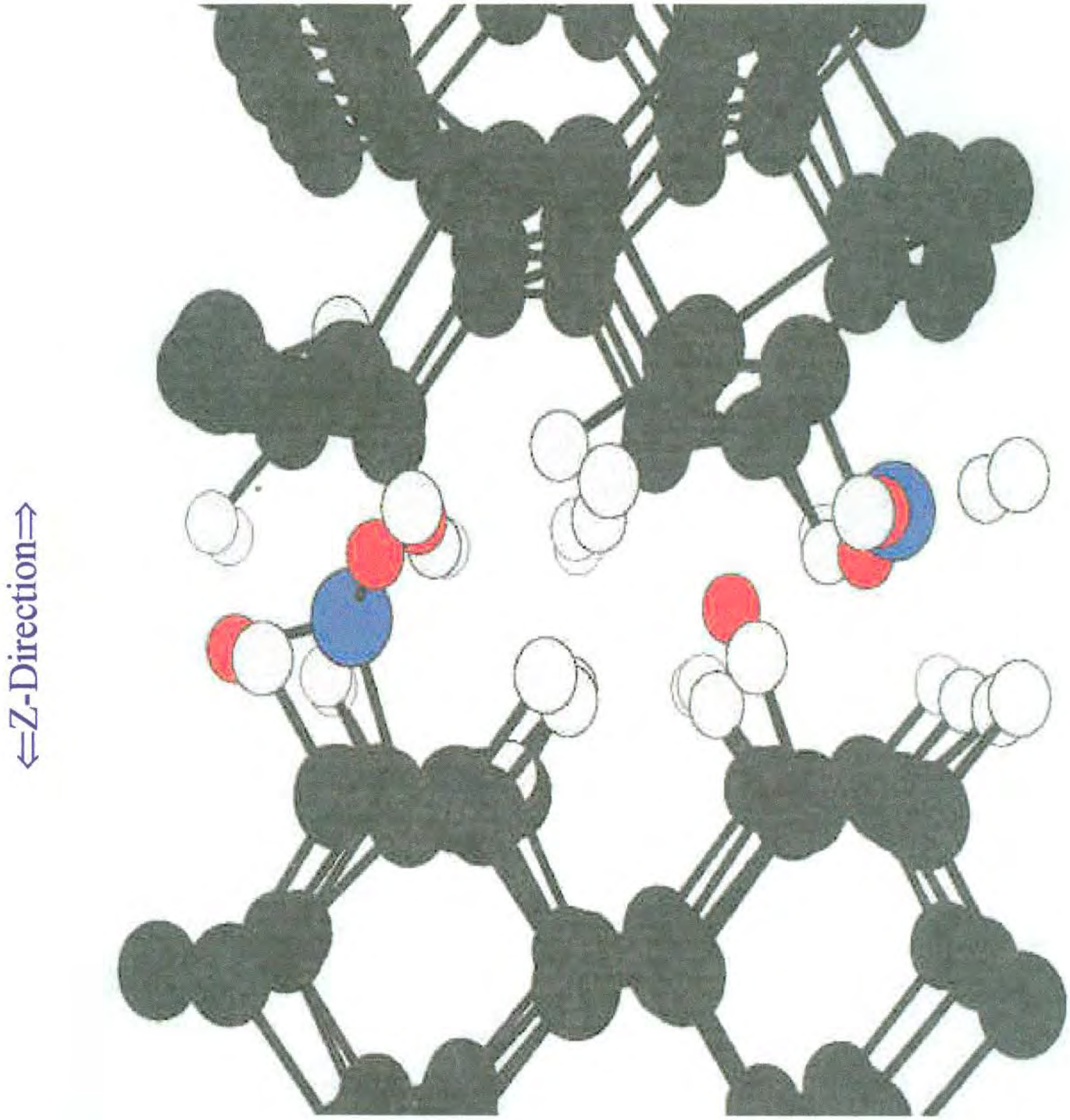


Figure 57