

# Ch 121a HW 4

Patryk Kozlowski

May 10, 2023

## 1 Problem 1

### 1.0.1 Question

What relationships are made by reax to properly allow bonds to form and break? (HINT: read the abstract of the 2001 paper)

### 1.0.2 Answer

This forcefield uses two relationships to accomplish the proper dissociation of bonds. The first relationship is between bond distance and bond order. The second relationship is between bond order and bond energy. [1]

## 2 Problem 2

### 2.0.1 Question

It is common in md to use point charges – in 2023, this is unacceptable! The charge equilibration (QEq) method was an innovative implementation in which the charge was distributed over the size of the atom. What additional feature could improve charge distribution even further? (HINT: read the abstract from the paper linked here)

### 2.0.2 Answer

this paper suggest that taking into account experimental polarizabilities for individual atoms, in a scheme known as PQEq, Would improve charge distribution even further. [2]

### 3 Problem 3

#### 3.0.1 Question

At 100 K, at what velocity does the water fragment after impact?

#### 3.0.2 Answer

At 100 K, the water fragments into a hydroxide and proton at a velocity between 0.7 and 0.9 km/s.

### 4 Problem 4

#### 4.1 Part a

##### 4.1.1 Question

Calculate the classical kinetic energy of the water molecule at each simulated velocity in kJ/mol.

##### 4.1.2 Answer

At 4 km/s, the kinetic energy is 144.08 kJ/mol. At 5 km/s, the kinetic energy is 225.12500000000003 kJ/mol. At 7 km/s, the kinetic energy is 441.24500000000006 kJ/mol. At 9 km/s, the kinetic energy is 729.4050000000001 kJ/mol. At 11 km/s, the kinetic energy is 1089.605 kJ/mol. At 13 km/s, the kinetic energy is 1521.8450000000003 kJ/mol.

#### 4.2 Part b

##### 4.2.1 Question

Given that water's bond energy is 493 kJ/mol, at what velocity would you expect the water to fragment in an ideal situation?

##### 4.2.2 Answer

Between 7 and 9 km/s.

## 4.3 Part c

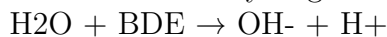
### 4.3.1 Question

Is this consistent with your simulations? If not, what non-ideality would cause this (there are several reasons for this so give it your best shot)?

### 4.3.2 Answer

Example: Hydrogen-Oxygen Bond in Water

BDE of water's hydrogen-oxygen bond is given by:



The above equation explains that when a water molecule is supplied with a certain amount of energy, it splits into two free radicals: H and OH.[3]

Using this definition, this was consistent with my simulations. The kinetic energy needed to separate the water molecule into a proton and hydroxide ion occurred between 7 and 9 km/s. The water molecule, also, did not fragment at 5 km/s at 300 K. I imagine that there should be some non-ideality, though, due to the fact that the water molecules are not in a vacuum, as there is some air friction involved, and so the fragmentation velocity would be closer to 9 km/s in actuality.

## References

- [1] Adri CT Van Duin, Siddharth Dasgupta, Francois Lorant, and William A Goddard. Reaxff: a reactive force field for hydrocarbons. *The Journal of Physical Chemistry A*, 105(41):9396–9409, 2001.
- [2] Saber Naserifar, Daniel J Brooks, William A Goddard III, and Vaclav Cvicek. Polarizable charge equilibration model for predicting accurate electrostatic interactions in molecules and solids. *The Journal of chemical physics*, 146(12):124117, 2017.
- [3] Turito. Bond energy - definition, factors, importance: Turito, Apr 2023.