CHEMISTRY EDUCATION AND COMPUTING

A COMPUTATIONAL APPROACH TO TEACHING INTRO TO CHEMISTRY

International School of Louisiana

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LA-SiGMA
Louisiana Alliance for Simulation-Guided Materials Applications

ABSTRACT

Chemistry is best taught using visual cues

- Research supports use of animation in teaching chemistry
- Experiment conducted in urban high school in Israel supports computerized modeling
- Students in the experimental group scored higher in the areas of;
    - Perception of models
    - Spatial ability
    - New concepts related to geometry and spatial ability
- In conjunction with the Chemistry Department at UNO, Gaussian View, VMD, Xmgrace and Amber Tools will be added to lesson plans

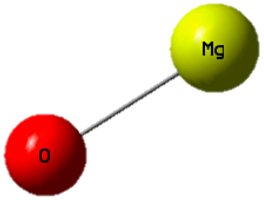
Barnea and Dori J. Sci. Edu. Tech. 1999 8 (4) 257-268

G-VIEW AS A TEACHING TOOL

Gview – students will practice building simple models.

- Differentiating between ionic and molecular bonding.
- Students must determine number of bonds.
- Students will be able to visualize the affects of forces by observing bond angles

Ex.



Magnesium Oxide

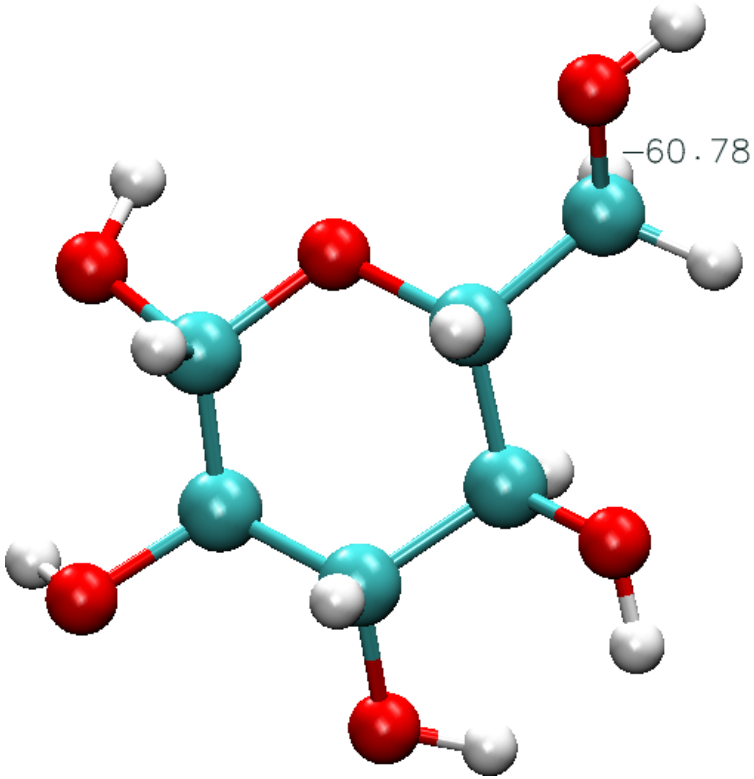
Gaussian View is a molecular building interface. Gaussian view allows its users to build molecules simply and interact with them in 3 dimensions by simply manipulating the mouse.

VMD AS A TEACHING TOOL

VMD- Visual Molecular Dynamics

- Visualize molecules in 3 dimensions
- Visualize mobility of structures
- Develop spatial understanding

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built in scripting

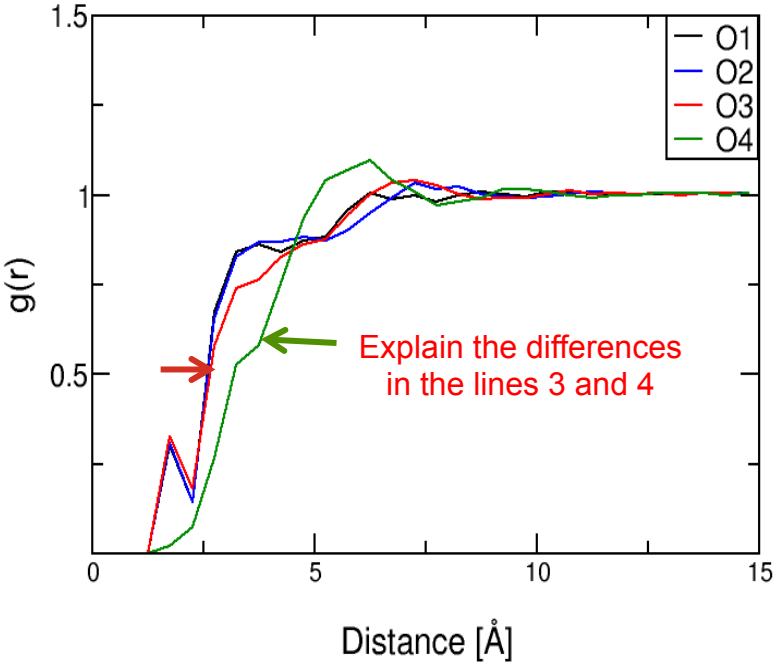


SIMULATIONS AS A TEACHING TOOL

Simulations using Amber tools, VMD and Xmgrace-

- visualize changes due to differences in solution and molecule
  - Focusing on RDF and h-bonding as a indicator of dissolution
- Amber tools gather data based on angles, dihedrals, distance, and hydrogen bond count
- Xmgrace will produce the graphs

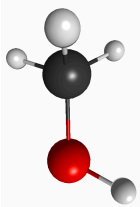
RDF Analysis



LESSON PLAN

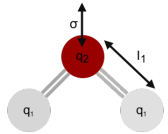
- Explain- structure of atoms, structure of bonds, types of bonds, nomenclature, van der Waals forces, polar molecules, atomic forces
- Engage- data will be collected experimentally
- Explore/Elaborate- data will be collected and analyzed computationally using VMD, Xmgrace, and Amber tools.
- Expound- compare experimental to computational

WORKFLOW

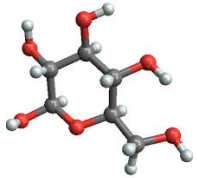


GPU enabled PMEMD
FF99SB and GLYCAM_06h
parameters

GPU enabled PMEMD
FF99SB and GLYCAM_06h parameters
SPC/E Water



Methanol



Aqueous solvent

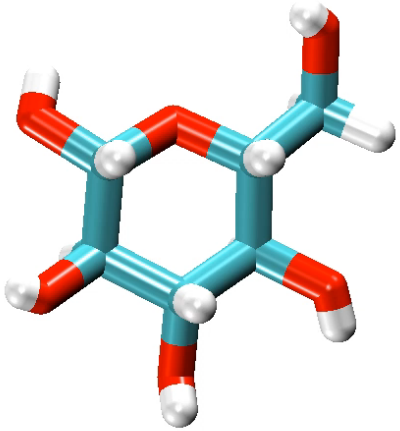
Glucose

Perform analysis using Cpptraj

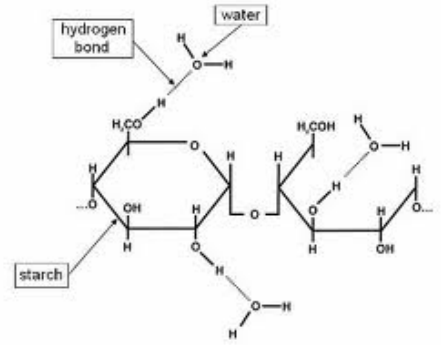
Xmgrace Graphing

VMD

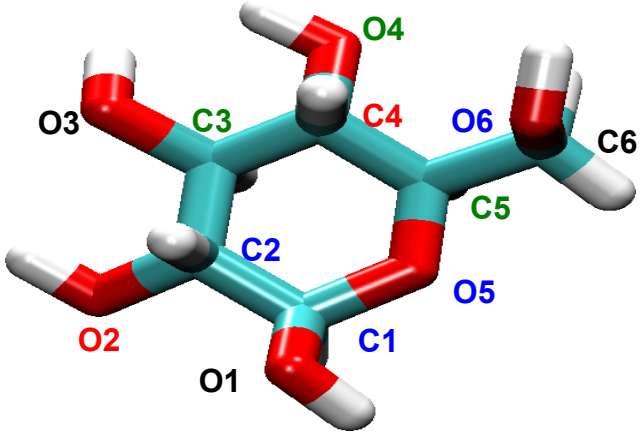
VMD Movie of Glucose Molecule in Water



Which carbons and oxygens have a better chance of interacting with the solvent? Why?

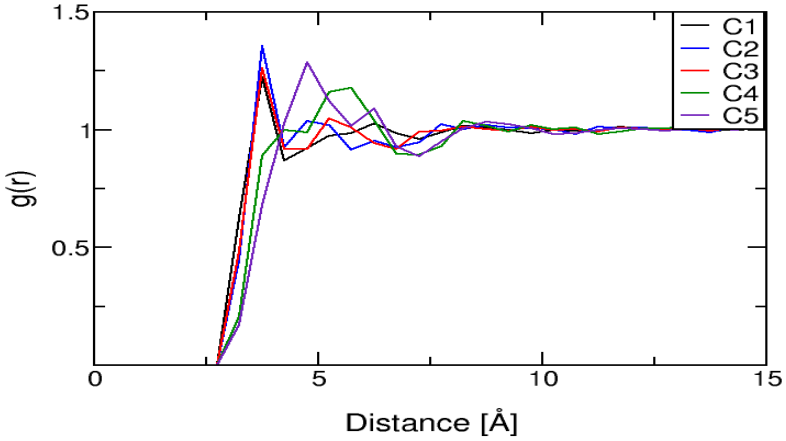


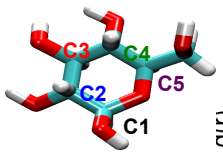
What type of bonds does glucose have the possibility of forming with water?



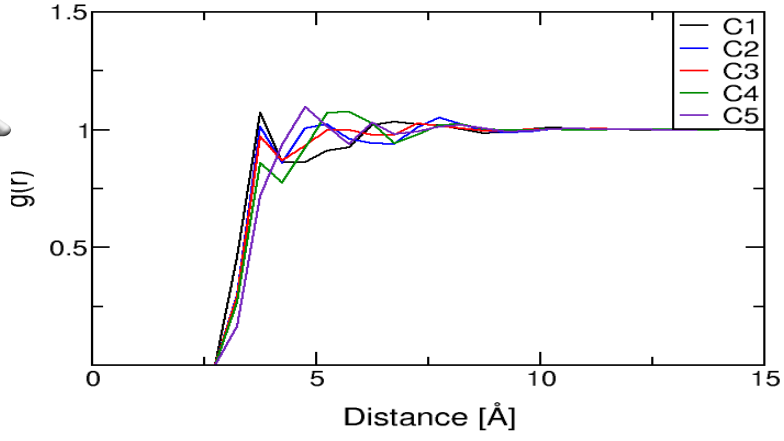
SIMULATION ANALYSIS CARBON

C – atom RDF - Methanol

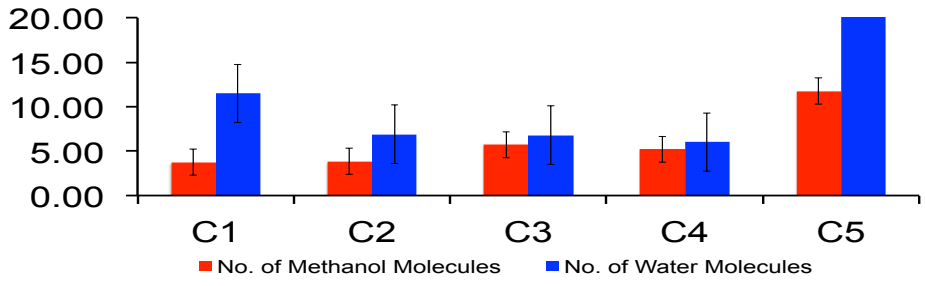




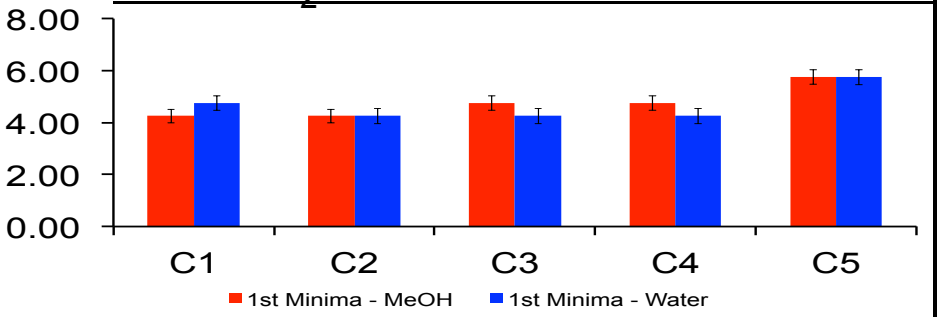
C – atom RDF – SPC/E Water



No. of MeOH/H_2O in 1st Minima

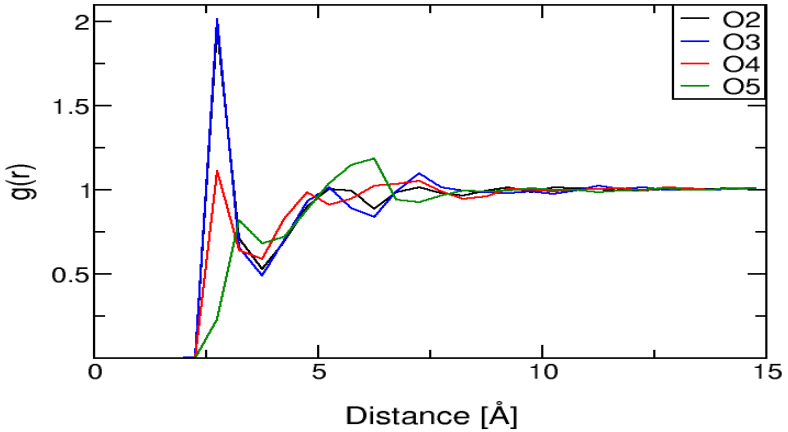


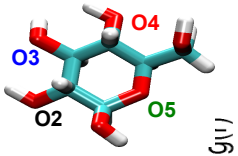
MeOH/H_2O 1st Minima around C- atom



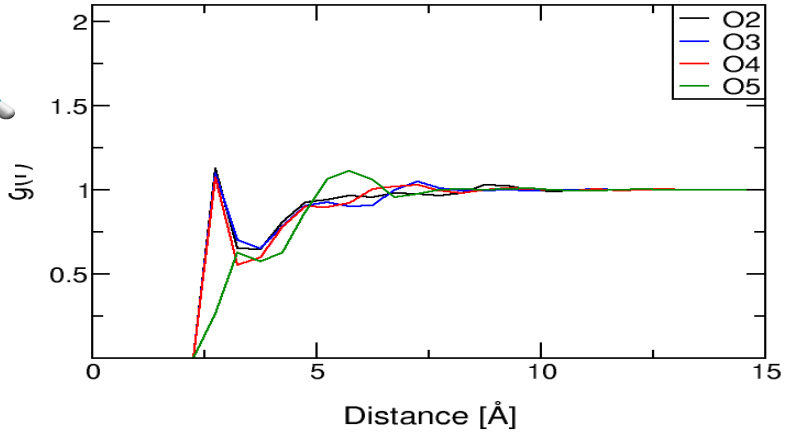
SIMULATION ANALYSIS OXYGEN

O – atom RDF - Methanol

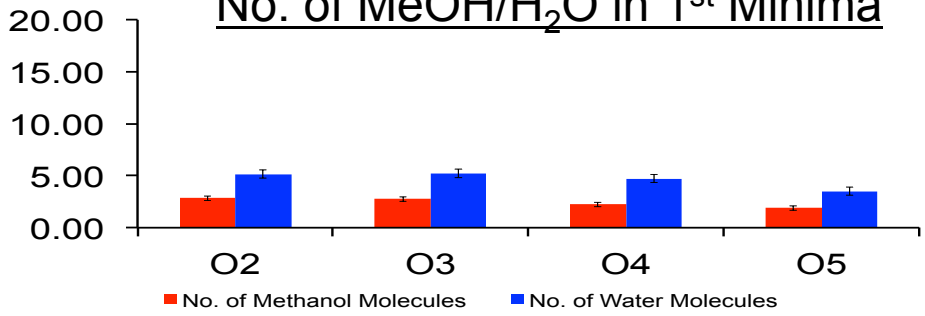




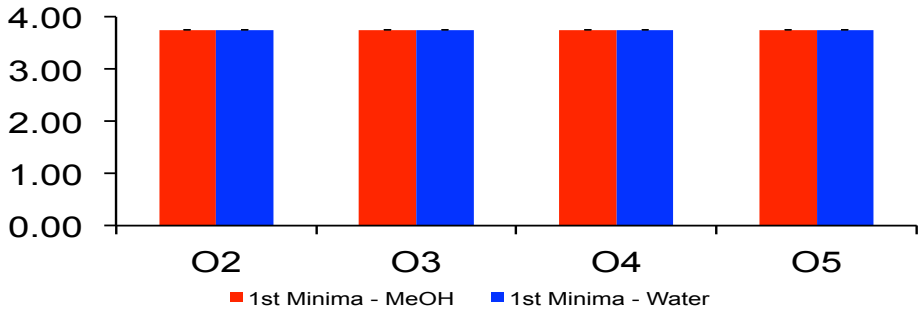
O – atom RDF – SPC/E Water



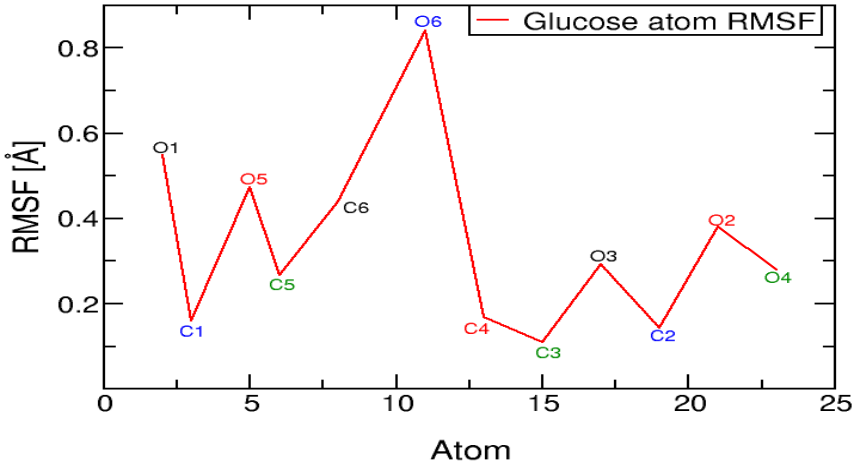
No. of MeOH/H_2O in 1st Minima



MeOH/H_2O 1st Minima around O- atom



RMSF of Glucose Molecule in Methanol



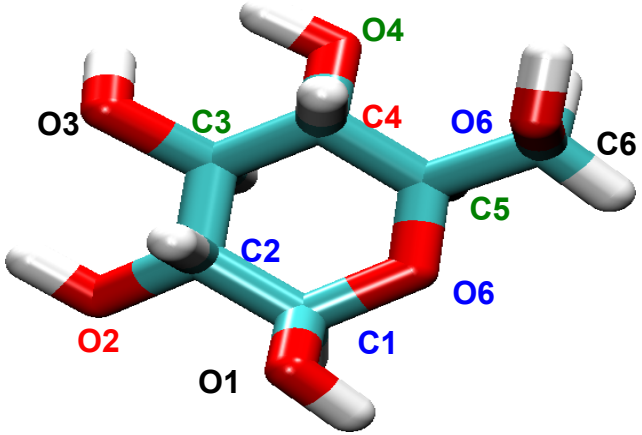


Table showing No. of MeOH and Water Molecules in 1st Minima of C - atoms

Glucose Atoms		
	No. of Methanol Molecules	No. of Water Molecules
C1	3.76	11.50
C2	3.84	6.89
C3	5.72	6.79
C4	5.23	6.04
C5	11.74	23.53

Table showing 1st Minima position around C - atoms

Glucose Atoms		
	1st Minima - MeOH	1st Minima - Water
C1	4.25	4.75
C2	4.25	4.25
C3	4.75	4.25
C4	4.75	4.25
C5	5.75	5.75

Table showing No. of MeOH and Water Molecules in 1st Minima of O - atoms

Glucose Atoms		
	No. of Methanol Molecules	No. of Water Molecules
O2	2.83	5.14
O3	2.76	5.21
O4	2.24	4.70
O5	1.90	3.50

Table showing 1st Minima position around O- atoms

Glucose Atoms		
	1st Minima - MeOH	1st Minima - Water
O1	3.75	3.75
O2	3.75	3.75
O3	3.75	3.75
O4	3.75	3.75

Students Analysis Continued..

#Distanc	Int[:2@C5]
0.250	0.000000
0.750	0.000000
1.250	0.000000
1.750	0.000000
2.250	0.000000
2.750	0.000000
3.250	0.365265
3.750	2.485109
4.250	6.021083
4.750	11.199980
5.250	17.040528
5.750	23.537304
6.250	31.973698
6.750	41.346024
7.250	52.272644
7.750	65.007880
8.250	79.539658
8.750	95.667383
9.250	113.418483
9.750	133.194555
10.250	155.215433
10.750	179.502610
11.250	206.051684
11.750	234.983216
12.250	266.400778
12.750	300.396786
13.250	337.113499
13.750	376.781496
14.250	419.308771
14.750	465.029168

Distance vs. Number of Water Molecules from vi

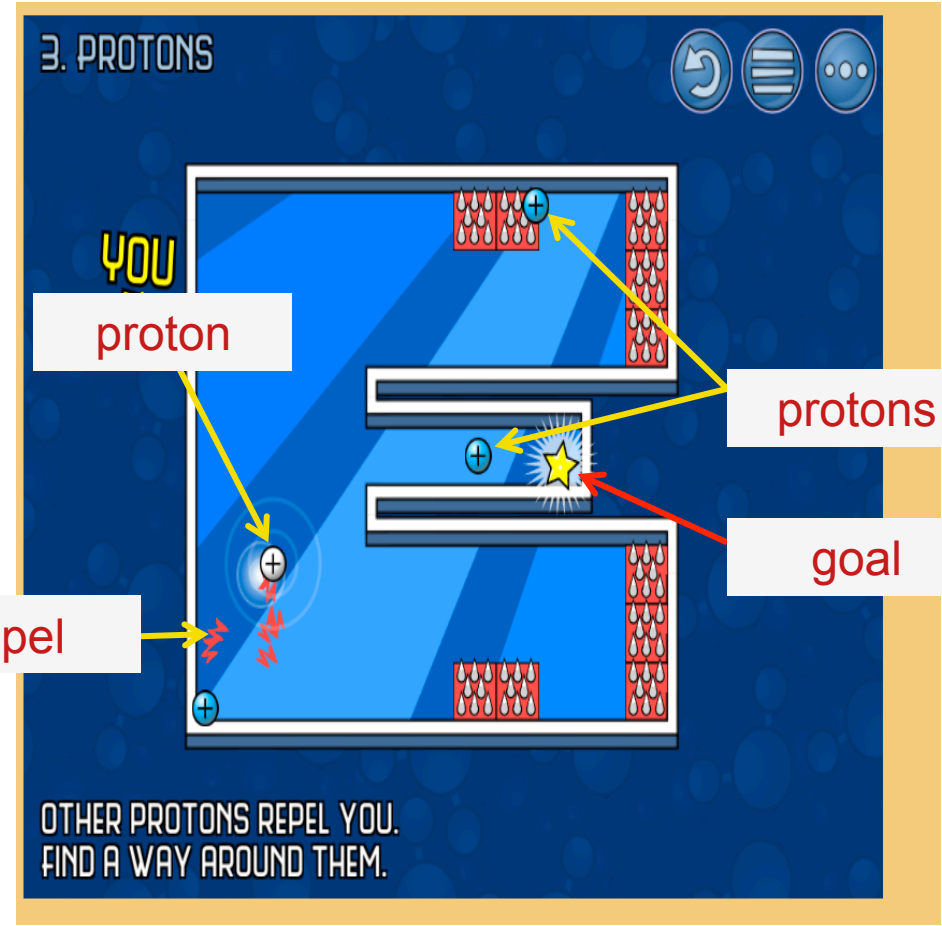
Students must create a graph for further analysis of distance versus interactions (RDF)

- Graph must have: title, labeling of the correct axis's, use of the correct type of graph (circle, bar, line)
- What conclusions can you draw about interaction of glucose in water? Is it different here than predicted?

ONLINE TOOLS

Bond Breaker

- Interactive game allows students to conceptualize forces inside atoms
  - Positive and negative
  - Van der Waals
  - Effects of heat on atoms



FUTURE WORK-COMPUTATIONAL

- Run the simulation for h-bonds in water and methanol
- RMSF-glucose in water
- VMD Movie for glucose in methanol
- Solvent accessible status
- Compare glucose and DPC RDF in water and methanol
- Analyze a different sugar-mannose and compare to data

FUTURE WORK

- **Connect with Donorschoose.org and other organizations to seek out funding for laptops capable of running viewing software as well as funding for licenses to run software**
- **Raspberrypi –Computers that can run the software**
- **QSM proposal for $750 towards materials**
- **Schedule UNO computer lab for school visit**
  - Approximately 55 students
  - 2 Dates (Late September – Early October)
- **Coordinate possible mentors for students that are interested in molecular dynamics for 2015/16 GNOSEF entries**

ACKNOWLEDGMENTS

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