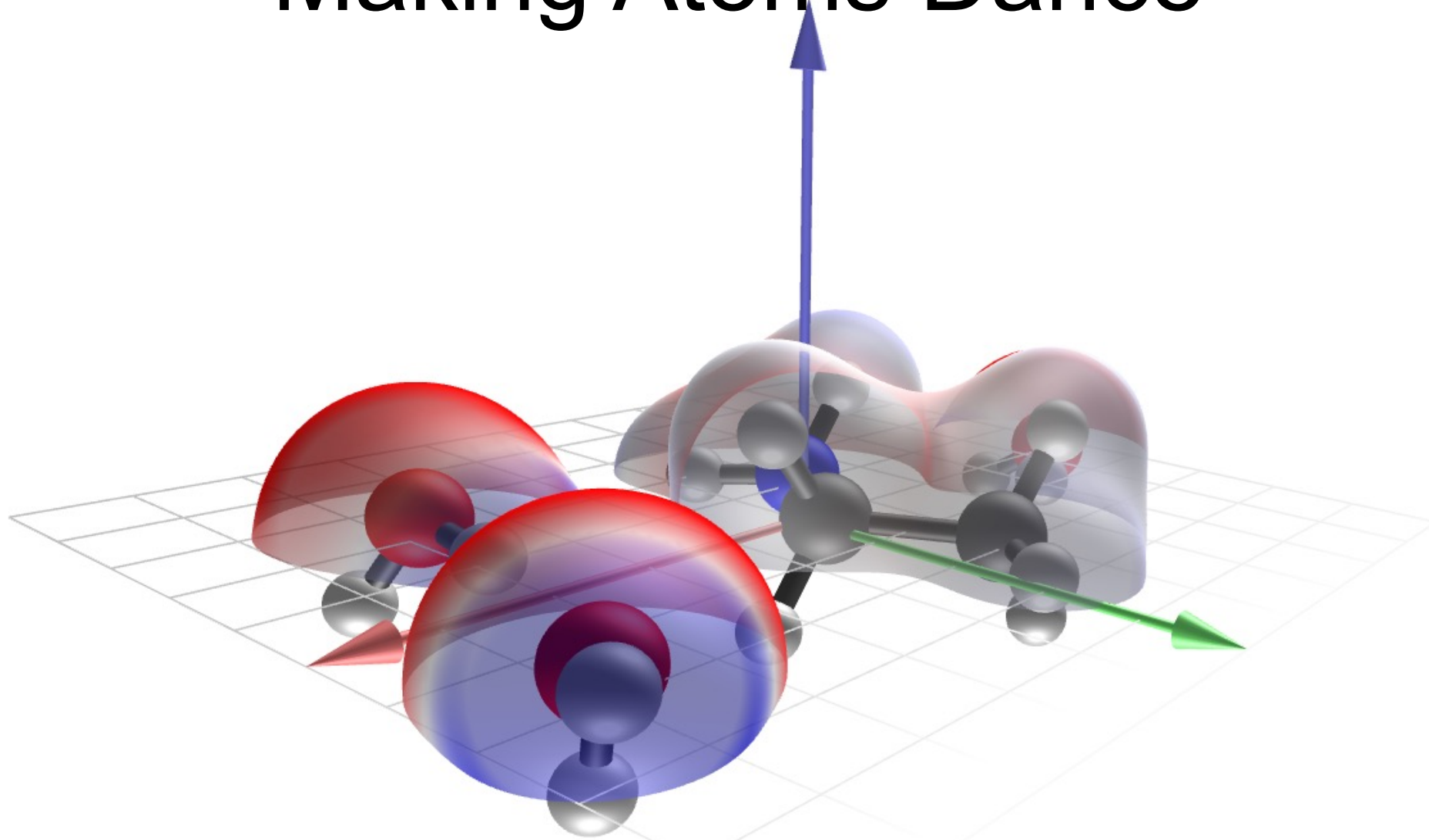


# Making Atoms Dance



Prof. Sudeep Bhattacharyay  
Department of Chemistry and Biochemistry  
Coordinator, Blugold High-performance Computing Center

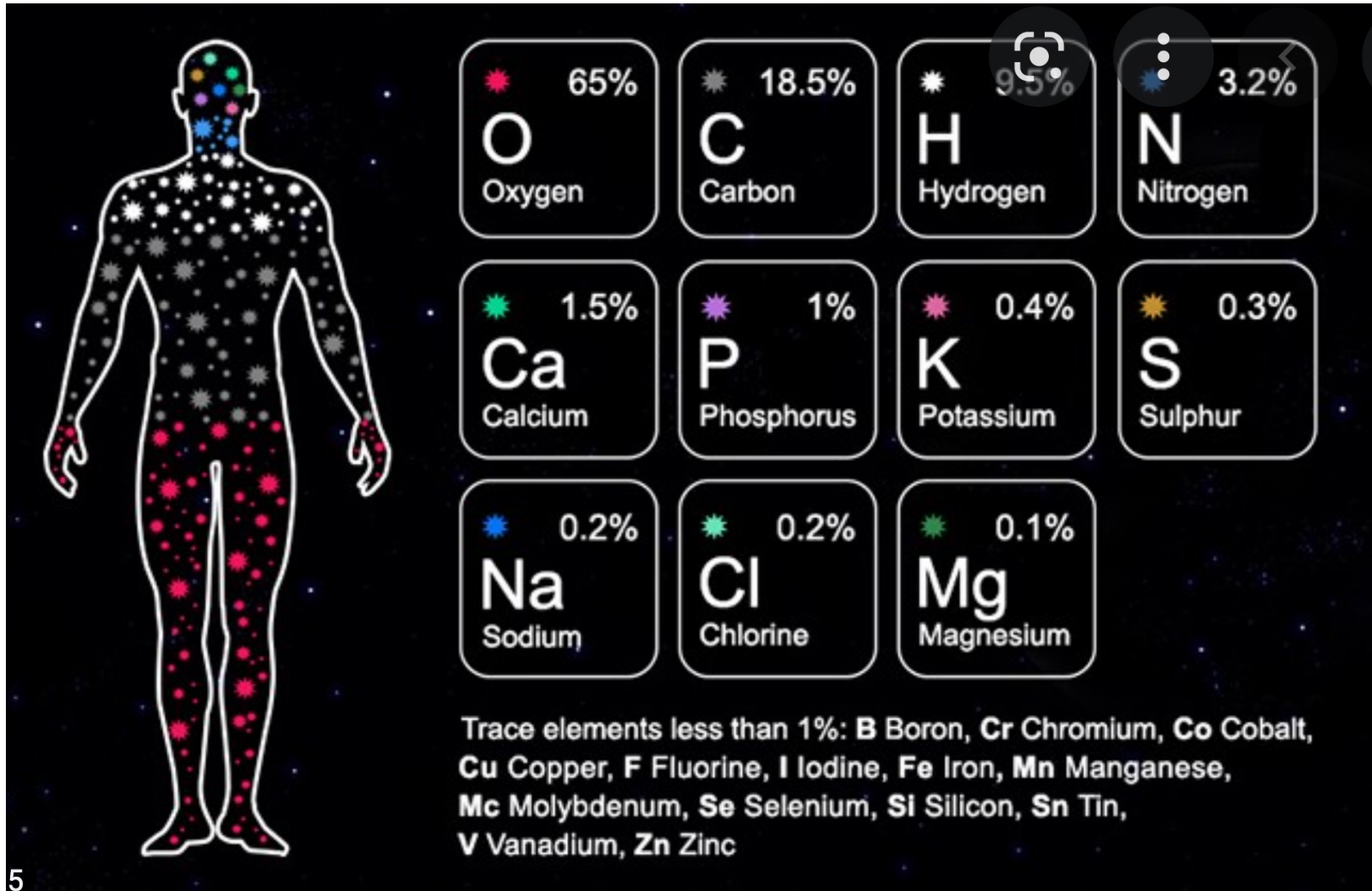
# Science and Our Universe

A photograph of a person standing on a rock in a dark landscape, looking up at the Milky Way galaxy in a starry night sky. The galaxy is visible as a bright, colorful band of stars and dust stretching across the sky. The person is silhouetted against the bright light of the galaxy.

We are made  
of **stardust**

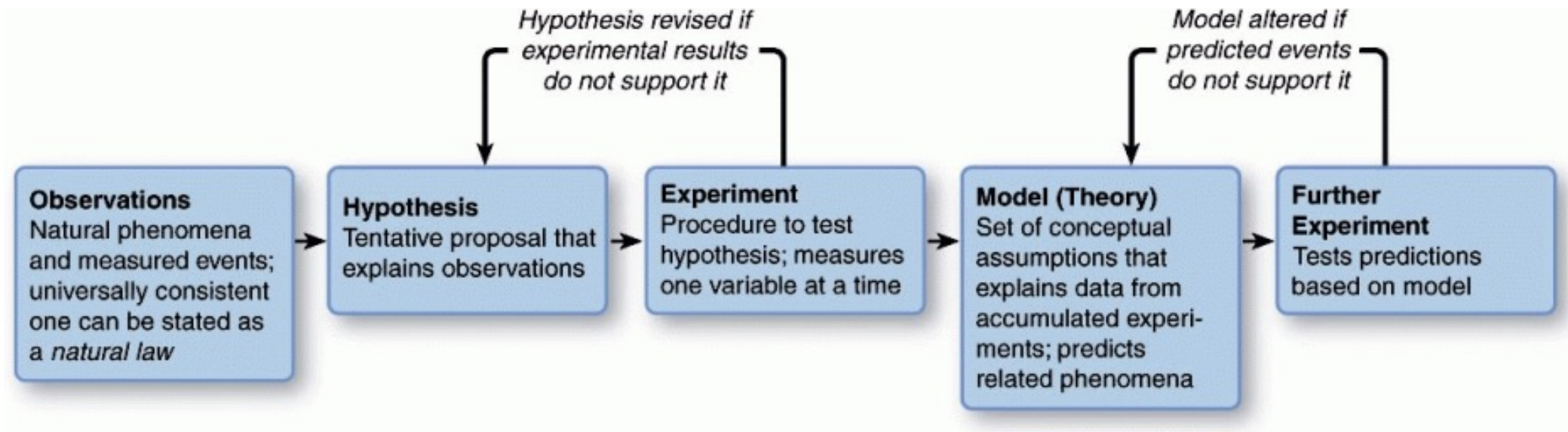
Nearly all of the  
elements of our body  
is made in a **star**

# Science and Our Universe



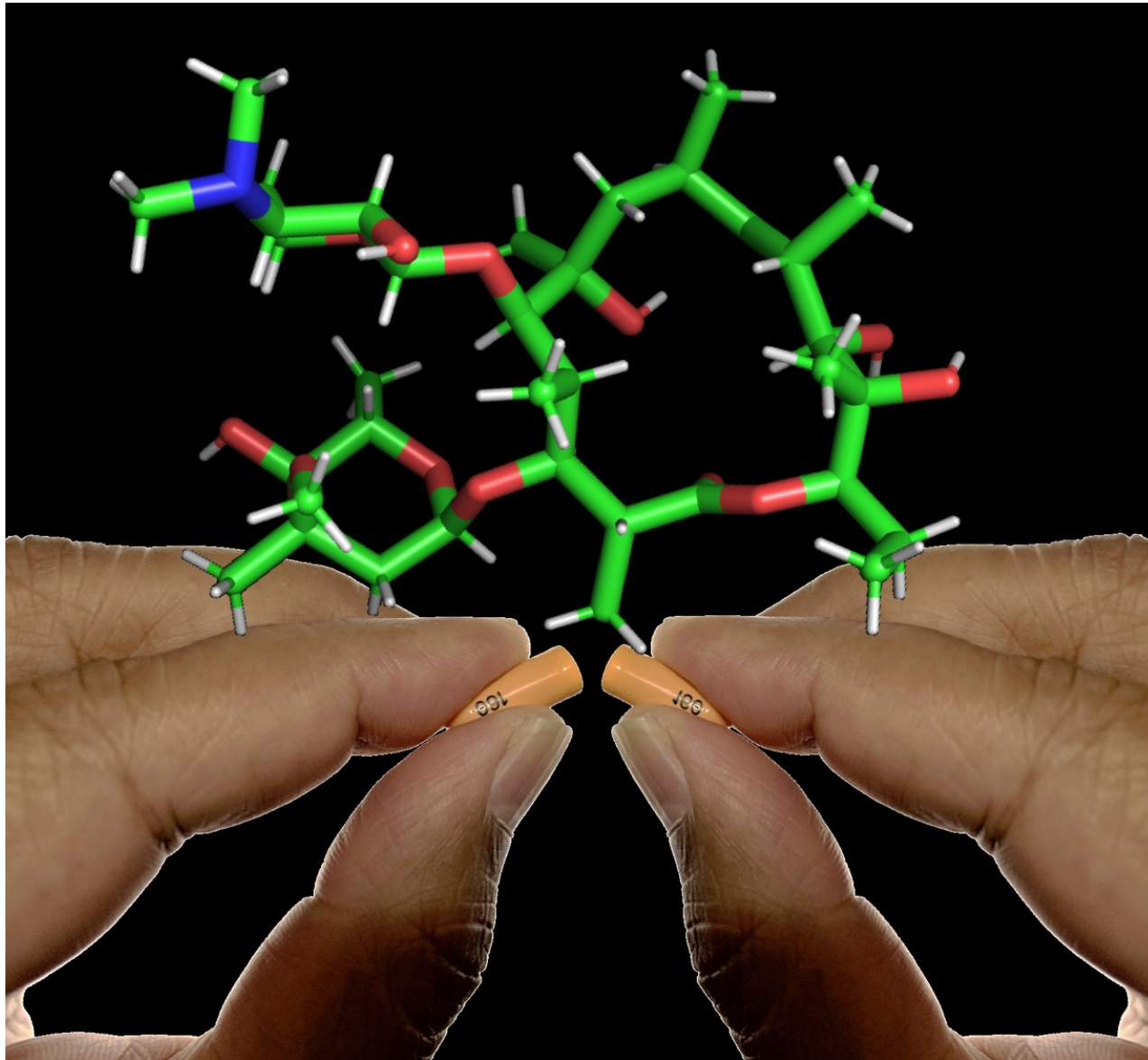
# The Scientific Method

- Scientists develop hypotheses, collect evidences from experiments, develop models, and then form a conclusion based on the results!



-An evidence-based understanding of the natural world

# Scientists are Explorers



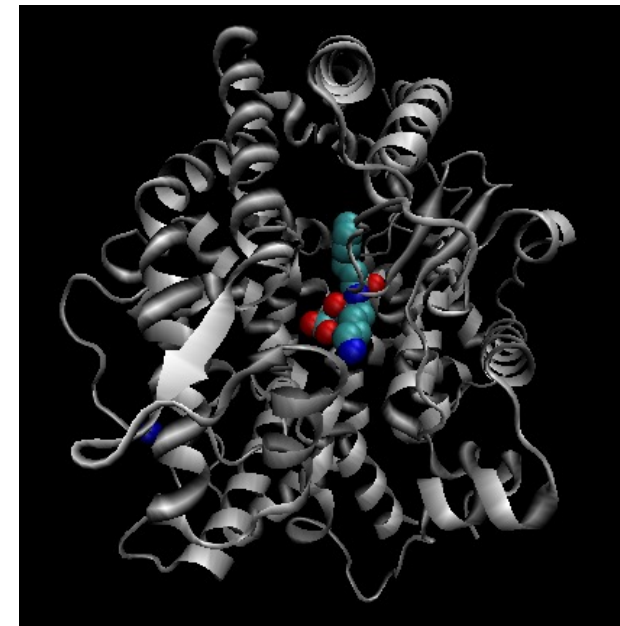
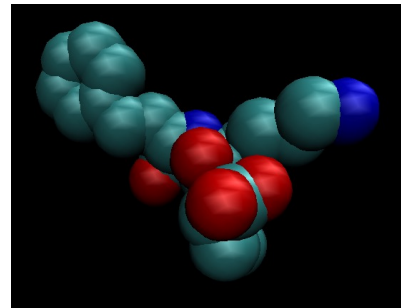
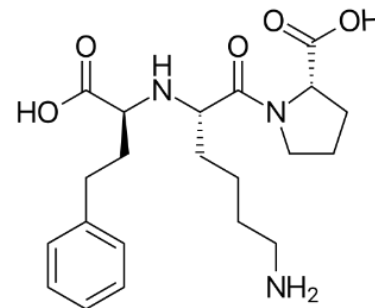
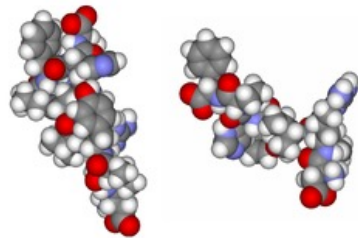
# Scientists are Explorers

Snake Venom to Drug (MERCK & Co)!!!!



- **Captopril, lisinopril**
- Treatment of high blood pressure
- ACE inhibitor (Angiotensin converting enzyme)
- From snake venom to ACE inhibitor — the discovery and rise of captopril

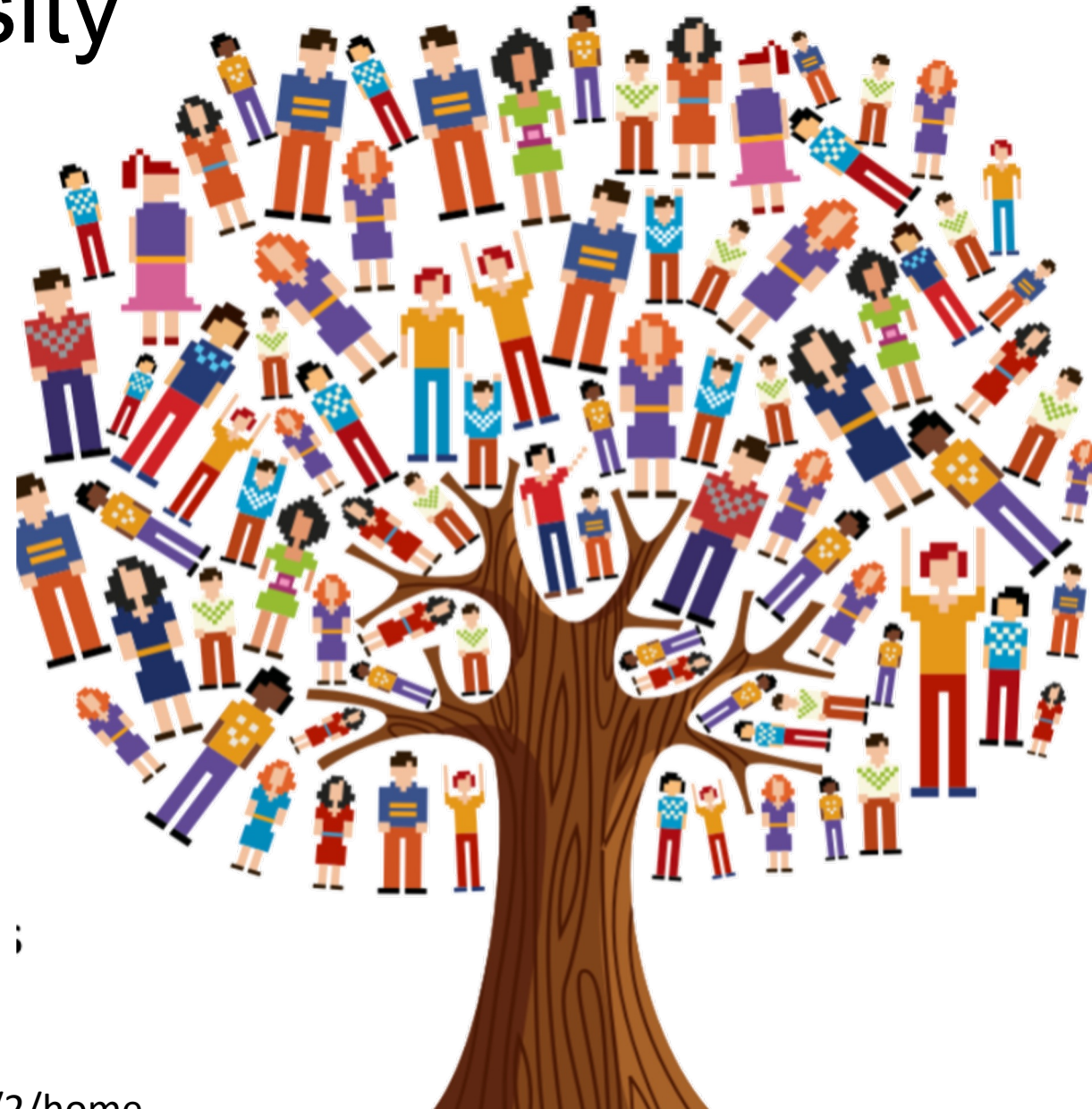
Angiotensin I



# Science Means Diversity

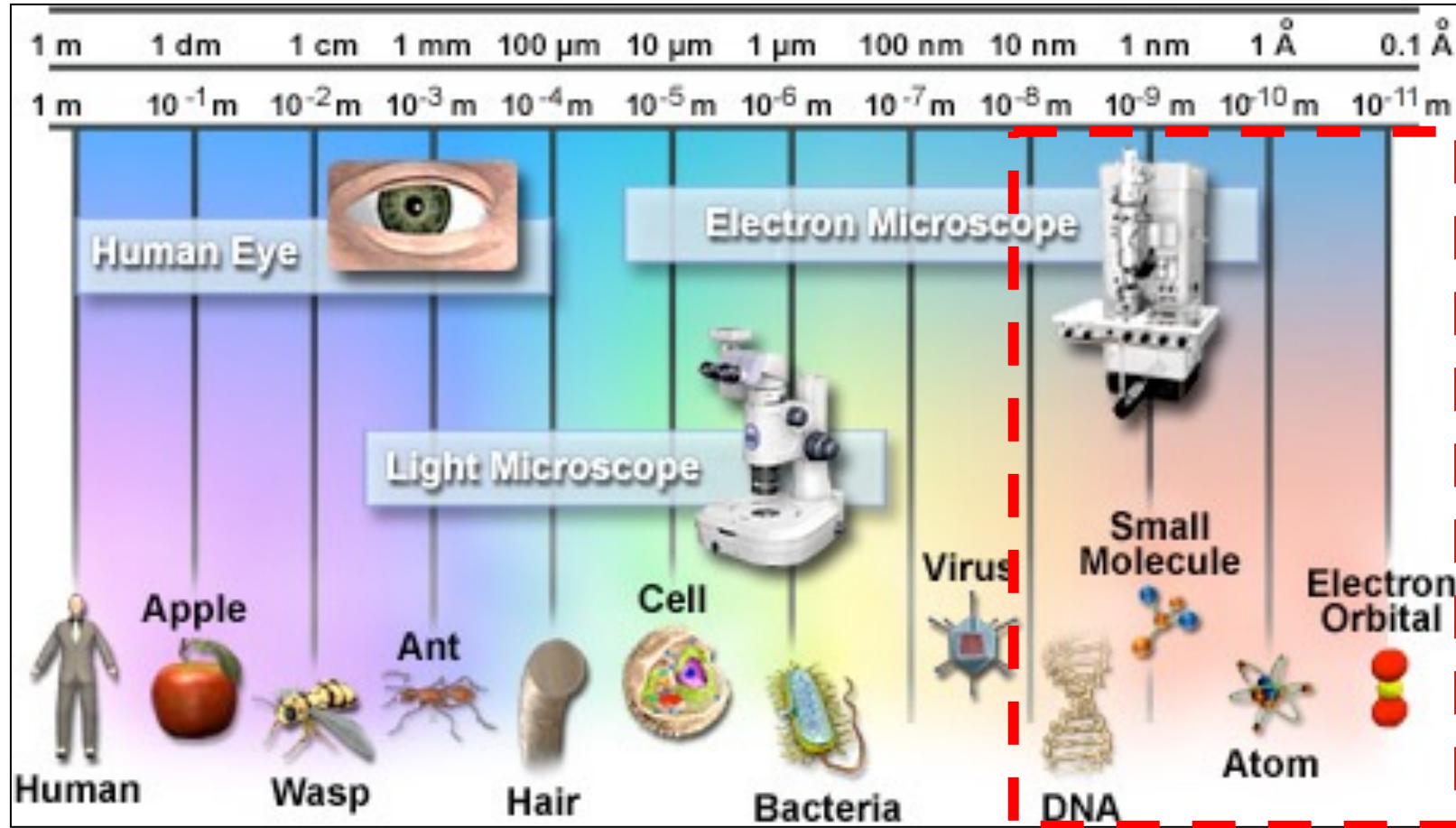
## Inclusion of the “other”

- Gender
- Race & Ethnicity
- Disabilities
- LGBTQIQA+
  - Lesbian
  - Gay
  - Bisexual
  - Transgender
  - Queer
  - Intersex
  - Questioning
  - Allies
  - Other Identities and orientation
- Socioeconomic
- Culture
- Life experiences
- Ideas
- Political Ideologies
- Religion
- Geography
- University Pedigrees
- Place of Origin
- Etc.



# The Science of Small Particles

## Relative Sizes and Detection Devices





# The Science of Small Particles

Higher or Normal mass

Particle nature

- ❑ Can have distinct mass and velocity
- ❑ Their vibrations can produce waves

Lower mass

Quantum nature

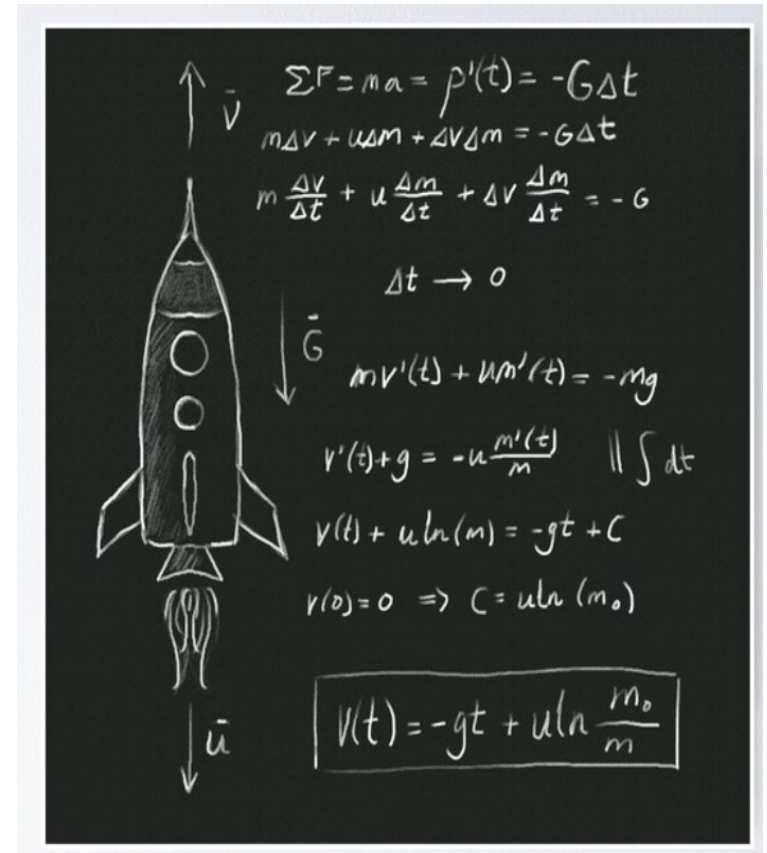
- ❑ Quantized energy levels
- ❑ Wave-particle duality

CHEMISTRY

# The Science of Small Particles

## Large objects

- ❑ Classical mechanics to predict the motion objects and understand waves
- ❑ We can adapt to the behavior as they are predictable



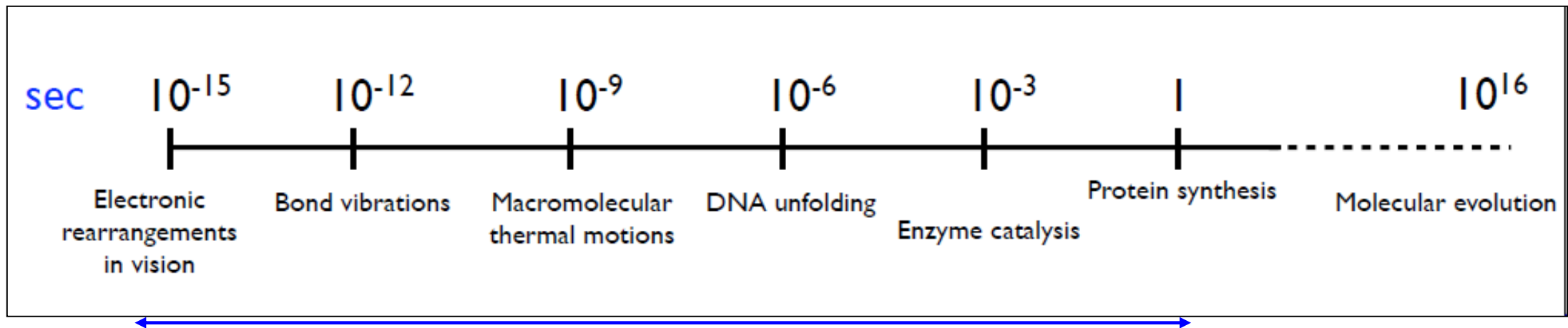
# The Science of Small Particles

## Too small objects

- ❑ Quantum mechanics to predict the motion
- ❑ Probabilistic interpretation of physical properties
- ❑ Fast dynamics

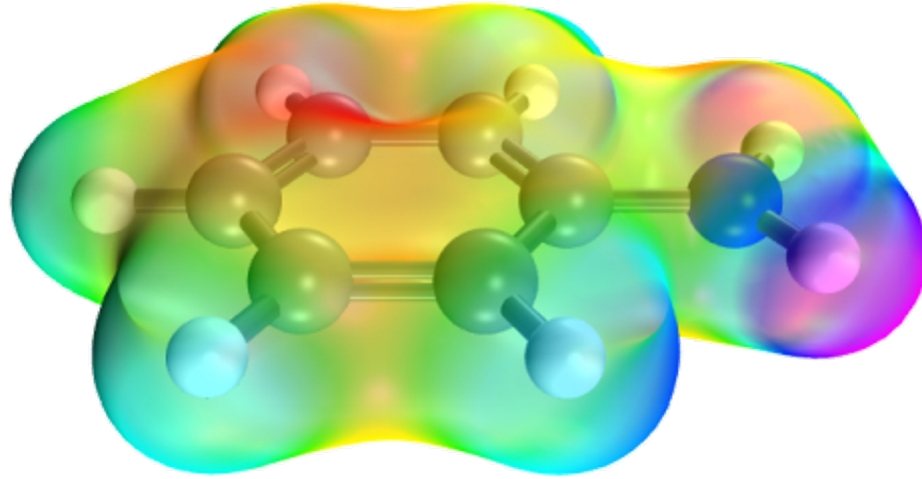
# The Science of Small Particles

## Timescales of various processes



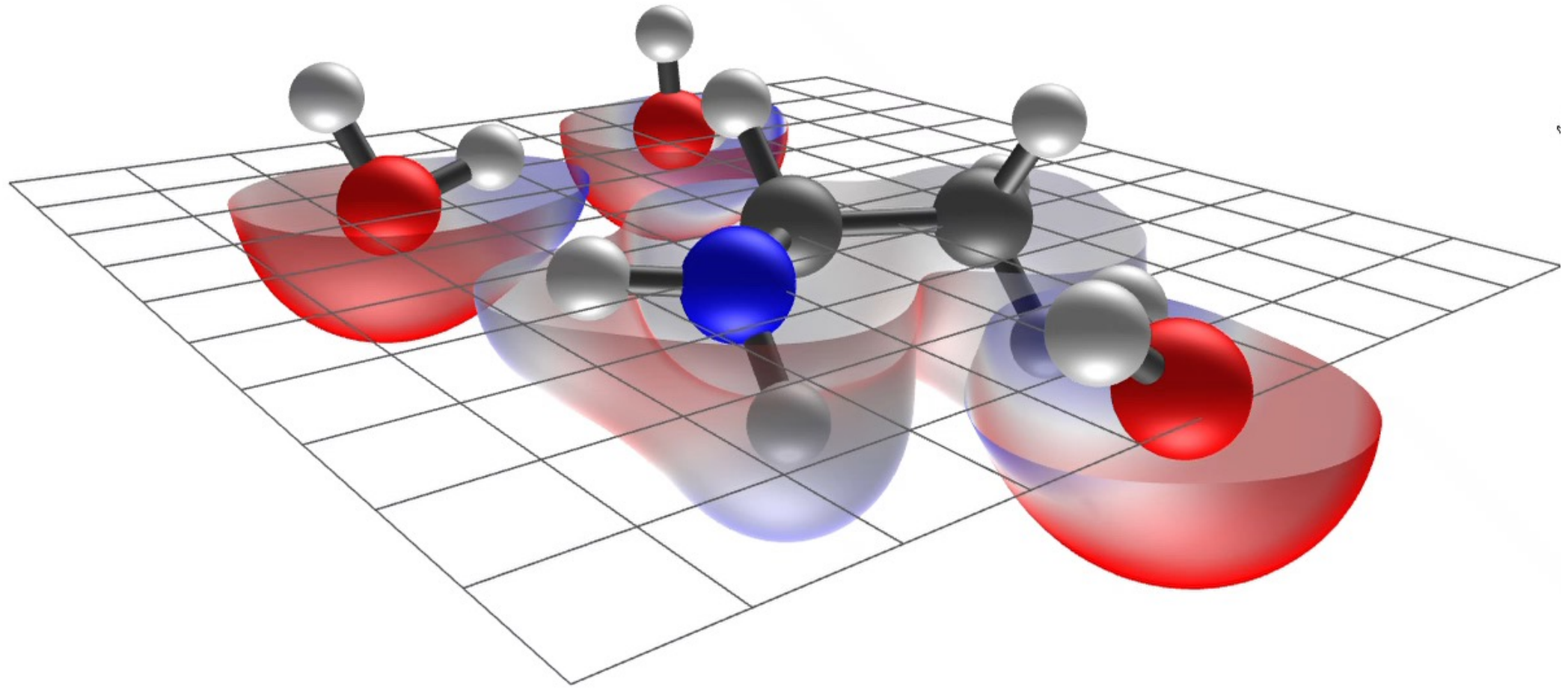
Chemistry

# Science of Changes - “Chemistry”

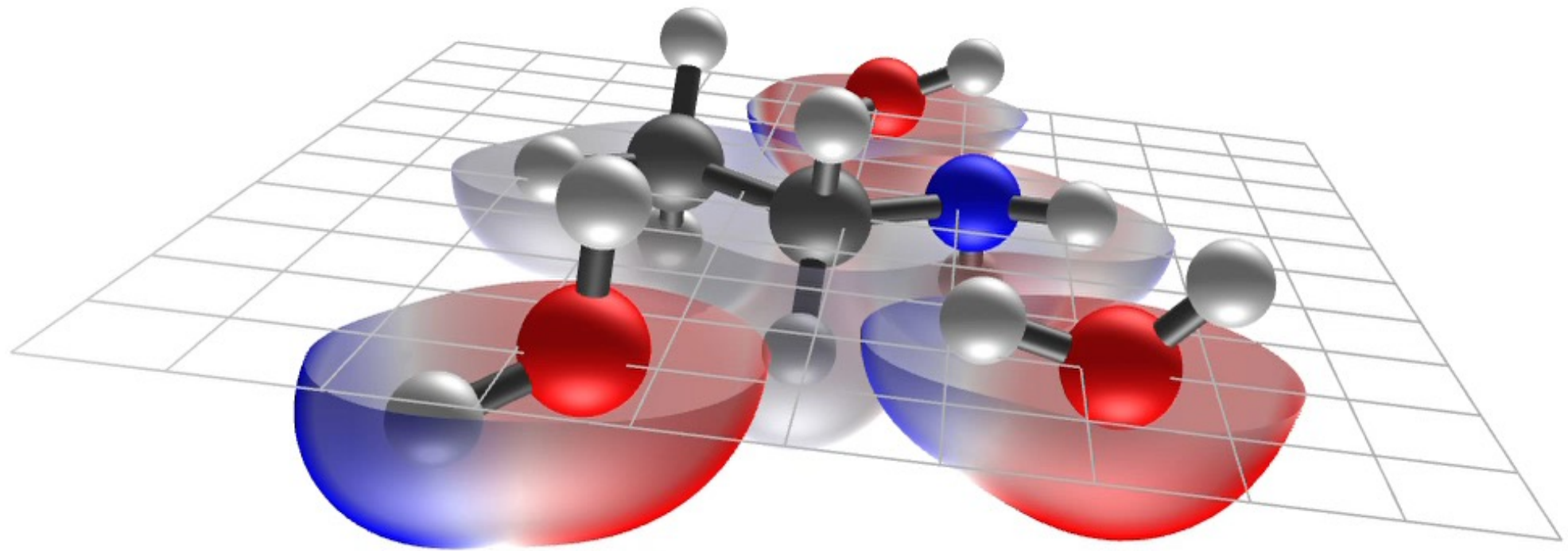


- Molecules are small and can not be seen under microscopes
- Made up of atoms
- Atoms are bonded by particles (electrons) which are even smaller
- Electrons are wave as well as particles
- Need quantum mechanics

# Science of Changes - “Chemistry”

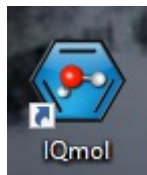


# Science of Changes - “Chemistry”



# Let us Build a Molecule

1. Open IQMol



2. Click once on the blue area to draw a single carbon atom, C

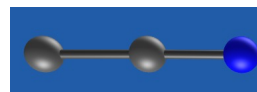
3. Click on the **carbon atom** and drag and release to draw the second bonded carbon atoms C-C



4. Now draw a 3<sup>rd</sup> atom, nitrogen. To do this, click on the build element 'C', open the periodic table and choose 'N'



4. (Use ctrl +z to undue a step if there is an error) and drag and release



5. Now, click on the 'N' and drag it to the next 'C' to draw the second bond and repeat this to draw third bond



6. Add hydrogens: Click the add hydrogen icon

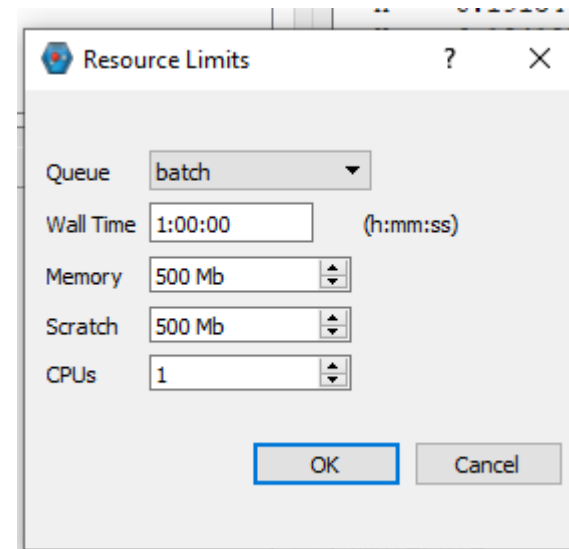




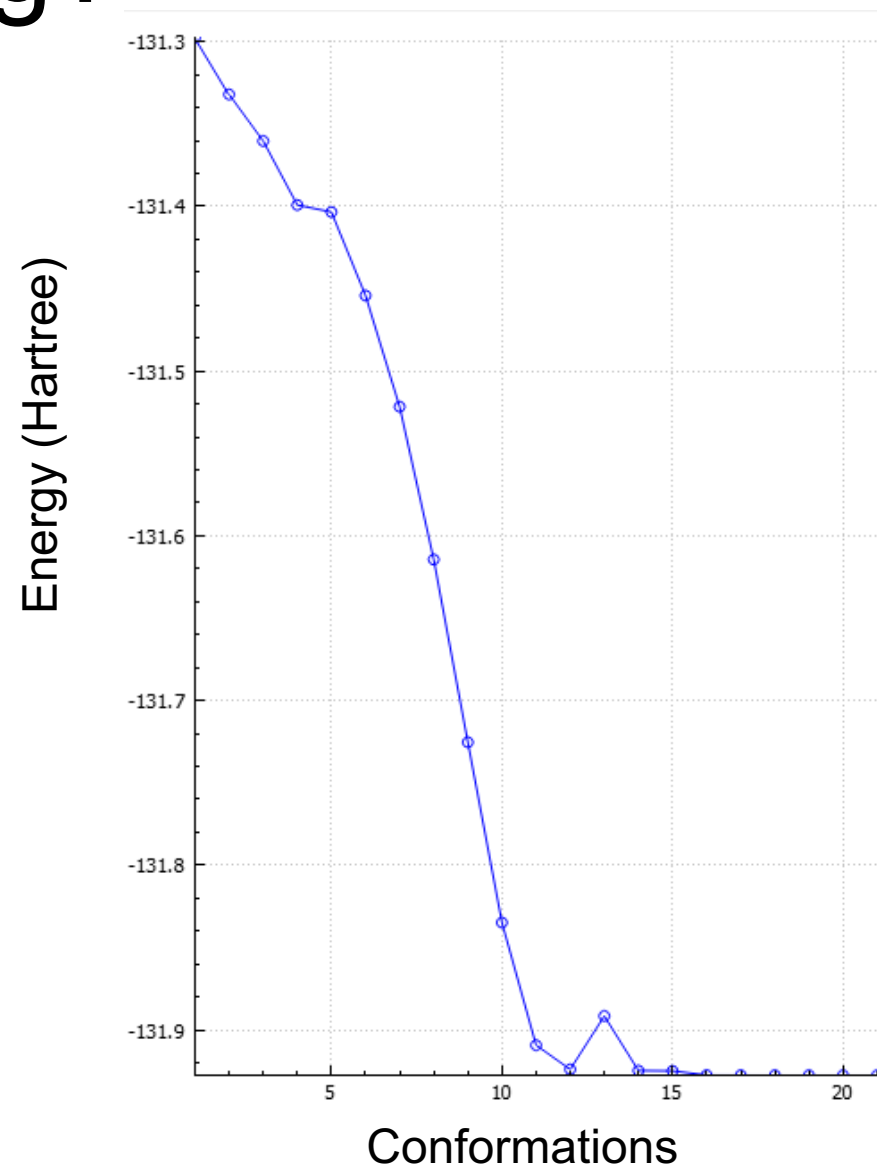
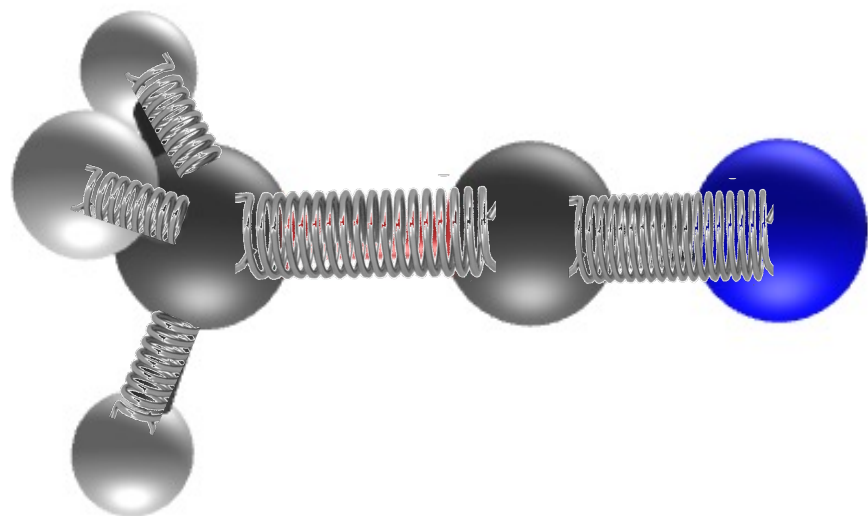
# Let us Calculate its Energy and Optimize

1. Open Calculation → Q-Chem Setup
  - a) Choose 'Geometry' for **Calculate**, 'HF' for **Method**, 6-31G\* for **Basis**
  - b) Click the '+' sign and choose 'Frequencies' for **Calculate**
  - c) Choose 'BGSC' for server and submit
  - d) You will see a popup window asking your password
  - e) Use 'mecn' as a new directory and use '1' as number of cores and hit 'ok'

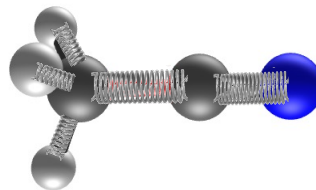
This will submit your calculation to **Blugold High-performance Cluster** computer.



# What is the Computer Doing?



# Bond Vibrations



Save the output files in a directory called 'mecn'

a) Open the mecn.out using IQMol

b) Double click "Geometries". Then look at the graph. Did energy rise or fall?

c) Click the 'play' button



d) Click the 'Global' to expand and choose select the 'Mesh' option

e) Double click the 'frequencies'

e) Click the 'play' button to see dancing of atoms

IQmol

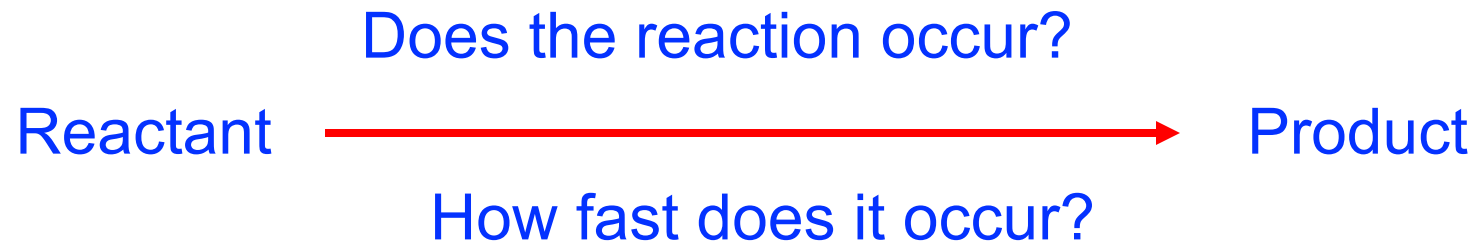
File Edit Display Build Calcu

Model View

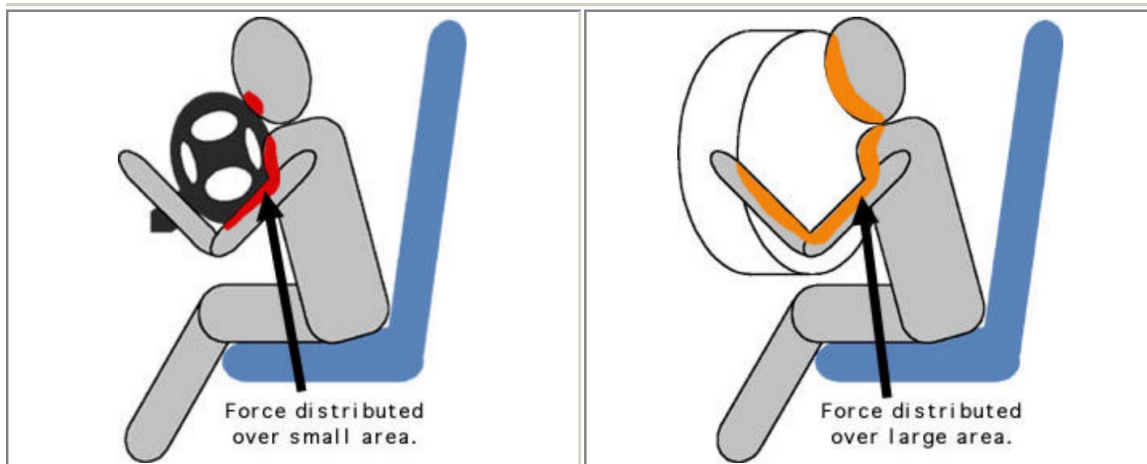
- ✓ Global
  - Background
  - Axes
  - Mesh
  - Clipping Plane
- ✓  mecn
  - > Info
  - > Files
  - > Atoms
  - > Bonds
  - Surfaces
  - > Frequencies
  - > Geometries

# Bond Vibrations

Why are bond vibrations important? [Chemistry](#)



# Bond Vibrations and Speed of a Reaction

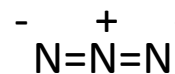


**Figure 5a**

When a body hits the steering wheel directly, the force of this impact is distributed over a small area of the body, resulting in injuries to this area. The area that hits the steering wheel is shown in red.

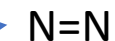
**Figure 5b**

When a body is restrained by an airbag, the force of the impact is distributed over a much larger area of the body, resulting in less severe injuries. The area that hits the airbag is shown in orange.



**Table 1**

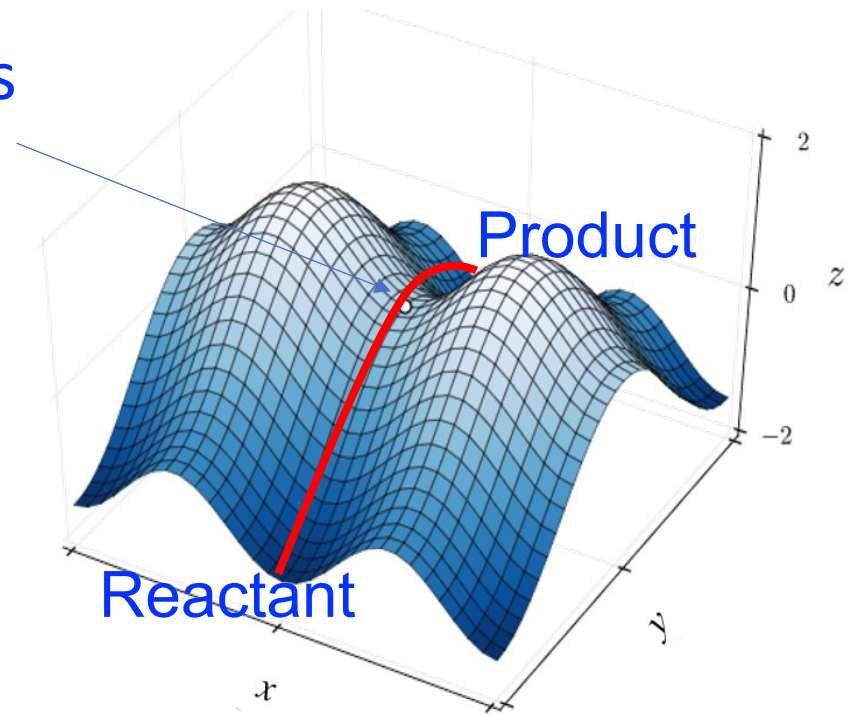
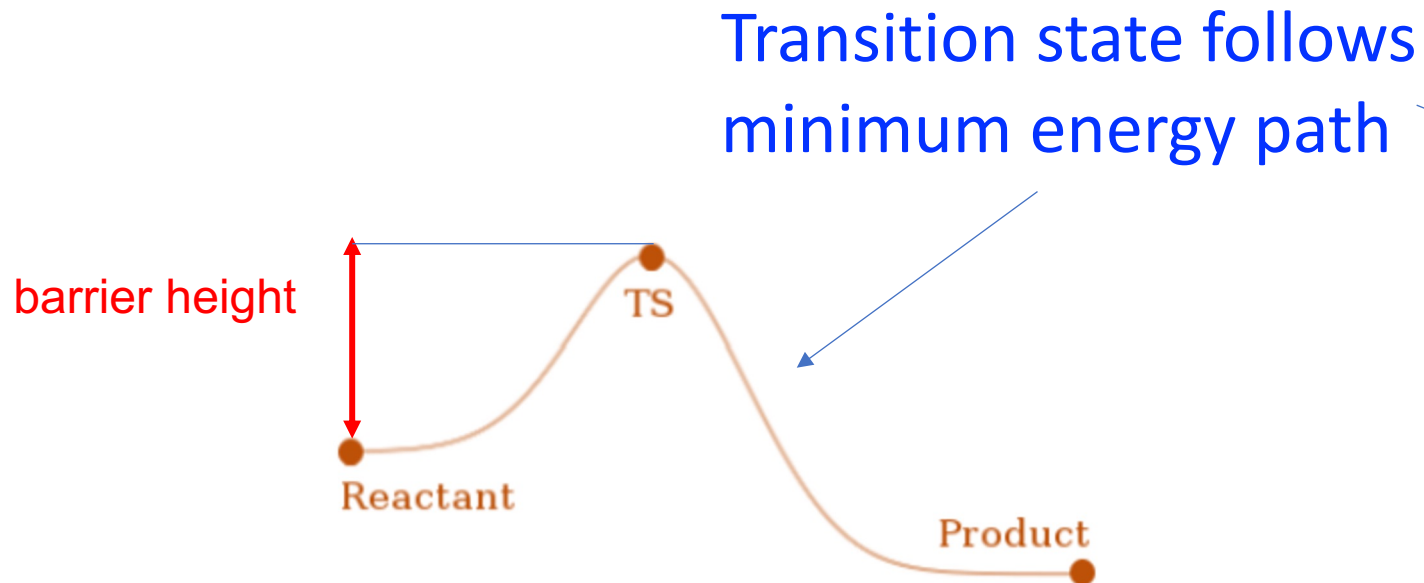
Gas-Generator Reaction	Reactants	Products
Initial Reaction Triggered by Sensor.	$\text{NaN}_3$	$\text{Na}, \text{N}_2 (\text{g})$
Second Reaction.	$\text{Na}, \text{KNO}_3$	$\text{K}_2\text{O}, \text{Na}_2\text{O}, \text{N}_2 (\text{g})$
Final Reaction.	$\text{K}_2\text{O}, \text{Na}_2\text{O}, \text{SiO}_2$	alkaline silicate (glass)



# Bond Vibrations and Speed of a Reaction

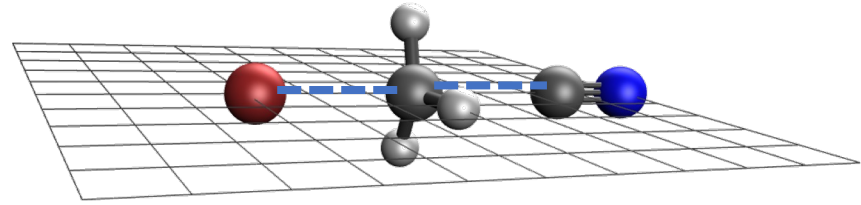
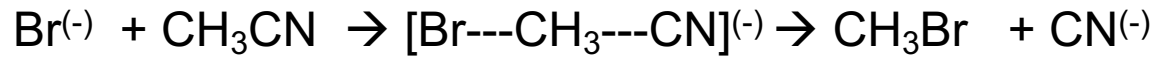
Transition state theory: Reacting molecules collide to produce a high-energy intermediate that has partially-formed bond

Taller the **barrier height** slower is the reaction




Only one imaginary frequency

# Bond Vibrations at the Transition State



Save the output files in a directory called 'mecn'

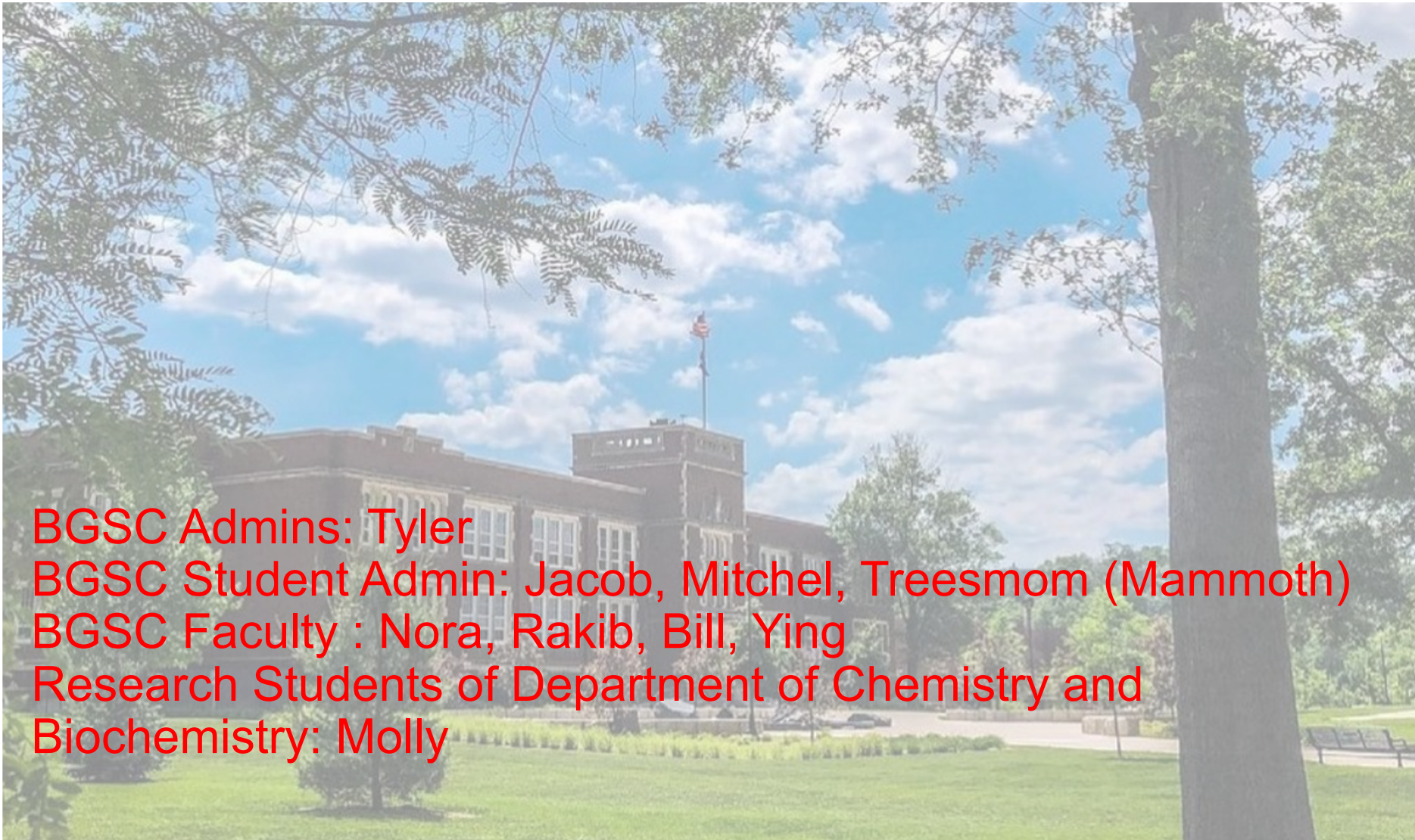
a) Open the ts\_geom\_freq.out using IQMol

b) Double click "frequencies". Click the 'play' button 

e) Click the 'play' button to see dancing of atoms

f) Which frequency corresponds to the bond breaking and bond forming?

# Acknowledgement



BGSC Admins: Tyler

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Research Students of Department of Chemistry and

Biochemistry: Molly