Excitement in Chemistry

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http://www.ncl.org.in/tcs/estg/spalhomepage.html

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“Science is organized and systematized knowledge relating to our physical world

Observation of phenomena as they occur in nature and their faithful recording

As the observations multiplied, regularities were sought and the facts were systematized. Formulation into laws, capable of embracing a number of facts and of summarizing them in succinct form with predictive power, these laws became theory. By comparison with experiments theories can be refined and new principles discovered” .

Scientific method or temper

Correlation of facts or explanation of qualitative information. Quantification and understanding in terms of laws and objectivity

Combination of experiment and theory using the scientific method has led to the development of present science.

Chemistry: Study of substances, their properties, structures and transformations. Synthesis of molecules of great complexity

Chemistry

- Chemistry is the study of matter and interactions between them.
- Chemistry and Physics are closely related. (chemical Physics)
- Chemistry tends to focus on the properties of substances and the interactions between different types of matter, involving study of electrons. Physics tends to focus more on the nuclear part of the atom, as well as the subatomic realm.

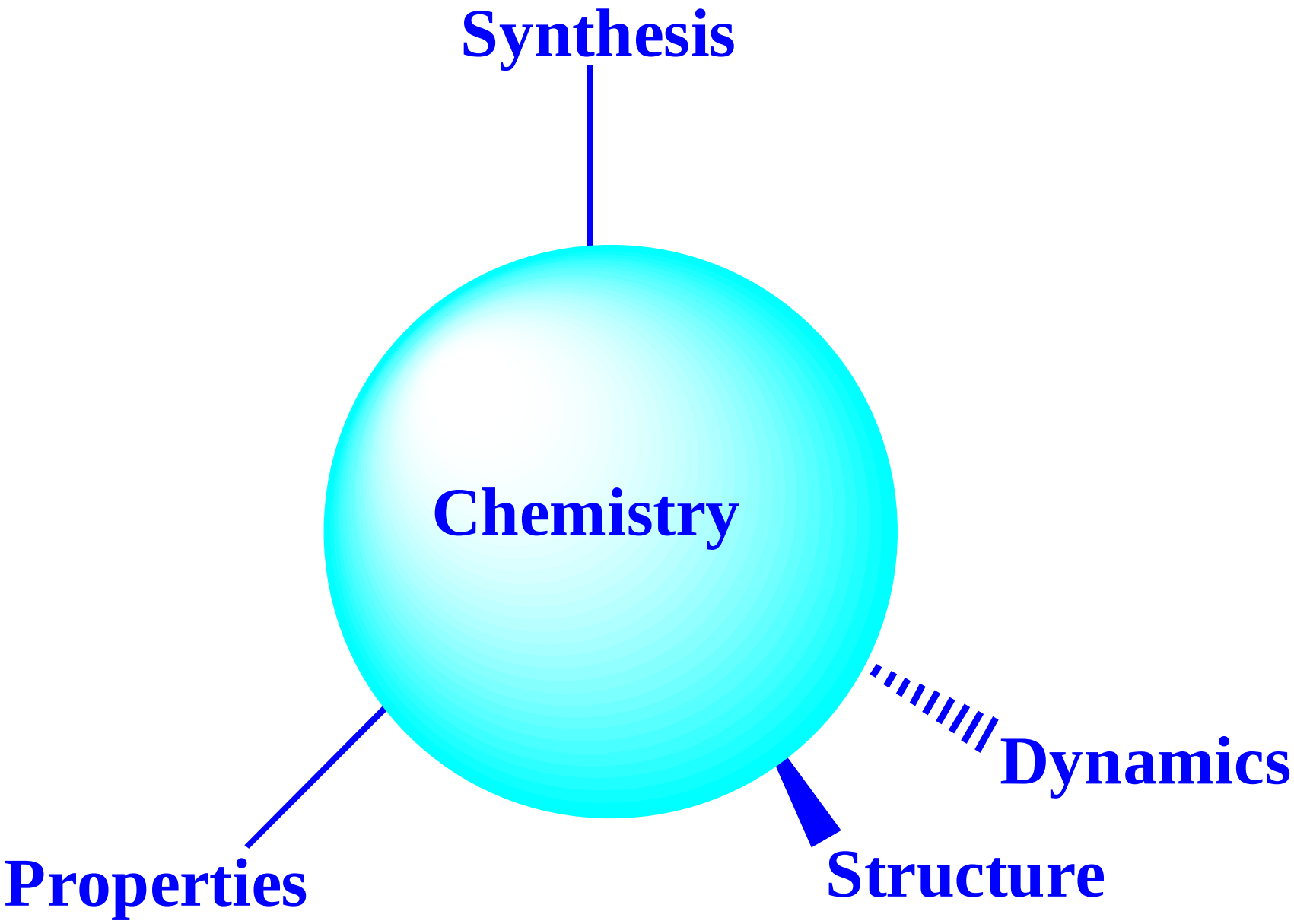
CHEMISTRY MOVES ON TWO WHEELS

CURIOSITY
UTILITY

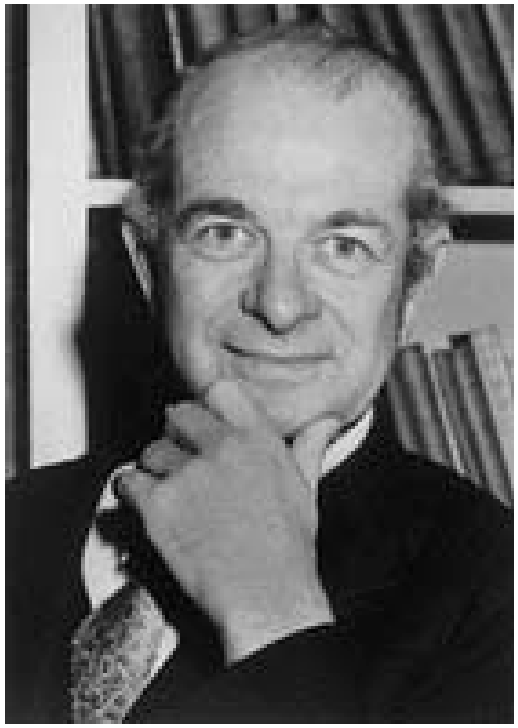
George Whitesides

What Fields of Study Use Chemistry

- Chemistry is used in most fields, but it's commonly seen in the sciences and in medicine. Chemists, physicists, biologists, and engineers study chemistry.
- Chemistry is the central science. Doctors, nurses, dentists, pharmacists, physical therapists, and veterinarians, fire-fighters all need chemistry. So do truck drivers, plumbers, artists, hairdressers, chefs... the list is extensive.


Synthesis
Chemistry
Dynamics
Properties
Structure

- Linus Pauling:



Nobel Prize:1954, 1962

his interest lay in the field of molecular structure and the nature of the chemical bond, inspired by papers by Irving Langmuir on the application of the Lewis theory of the sharing of pairs of electrons between atoms to many substances.

Linus Pauling's contributions: (downloaded from the web)

experimental determination of the structure of crystals by the diffraction of X-rays and the interpretation of these structures in terms of the radii and other properties of atoms; the application of quantum mechanics to physical and chemical problems, including dielectric constants, X-ray doublets, momentum distribution of electrons in atoms, rotational motion of molecules in crystals, Van der Waals forces, etc.; the structure of metals and intermetallic compounds, the theory of ferromagnetism; the nature of the chemical bond, including the resonance phenomenon in chemistry; the experimental determination of the structure of gas molecules by the diffraction of electrons; the structure of proteins; the structure of antibodies and the nature of serological reactions; the structure and properties of hemoglobin and related substances; abnormal hemoglobin molecules in relation to the hereditary hemolytic anemias; the molecular theory of general anesthesia; an instrument for determining the partial pressure of oxygen in a gas; and other subjects

G. N. Lewis (1875-1946)

G. N. Lewis:
Valence and the Structure of Atoms and Molecules

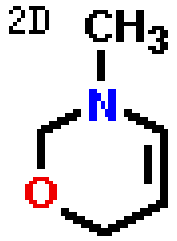
Lewis once defined physical chemistry as encompassing "everything that is interesting".*(3)*
“In his theory of the shared electron pair, Lewis did not believe only that an electron completely transfers from one atom to another, as in the positive-negative theory. He describes the partial transfer of two electrons, one from each of the two bonding atoms, so that there is a shared pair of electrons between them. This eliminates the need for the formation of oppositely charged atoms when there was no indication of individually charged atoms (ions) in a compound. This was the first description of covalent bonding.”

Ernest Rutherford

- Nobel Prize 1908 "for his investigations into the disintegration of the elements, and the chemistry of radioactive substances. His firsr research was concerned with the magnetic properties of iron exposed to high-frequency oscillations, and his thesis was entitled *Magnetization of Iron by High-Frequency Discharges*. During his first spell at the Cavendish Laboratory, he invented a detector for electromagnetic waves, an essential feature being an ingenious magnetizing coil containing tiny bundles of magnetized iron wire. He worked jointly with Thomson on the behaviour of the ions observed in gases which had been treated with X-rays, and also, in 1897, on the mobility of ions in relation to the strength of the electric field, and on related topics such as the photoelectric effect. In 1898 he reported the existence of alpha and beta rays in uranium radiation and indicated some of their properties

Michael Faraday (1791- 1867)

- Faraday's earliest chemical work was as an assistant to Davy. He made a special study of chlorine, and discovered two new chlorides of carbon. He also made the first rough experiments on the diffusion of gases, a phenomenon first pointed out by John Dalton, the physical importance of which was more fully brought to light by Thomas Graham and Joseph Loschmidt. He succeeded in liquefying several gases; he investigated the alloys of steel, and produced several new kinds of glass intended for optical purposes.

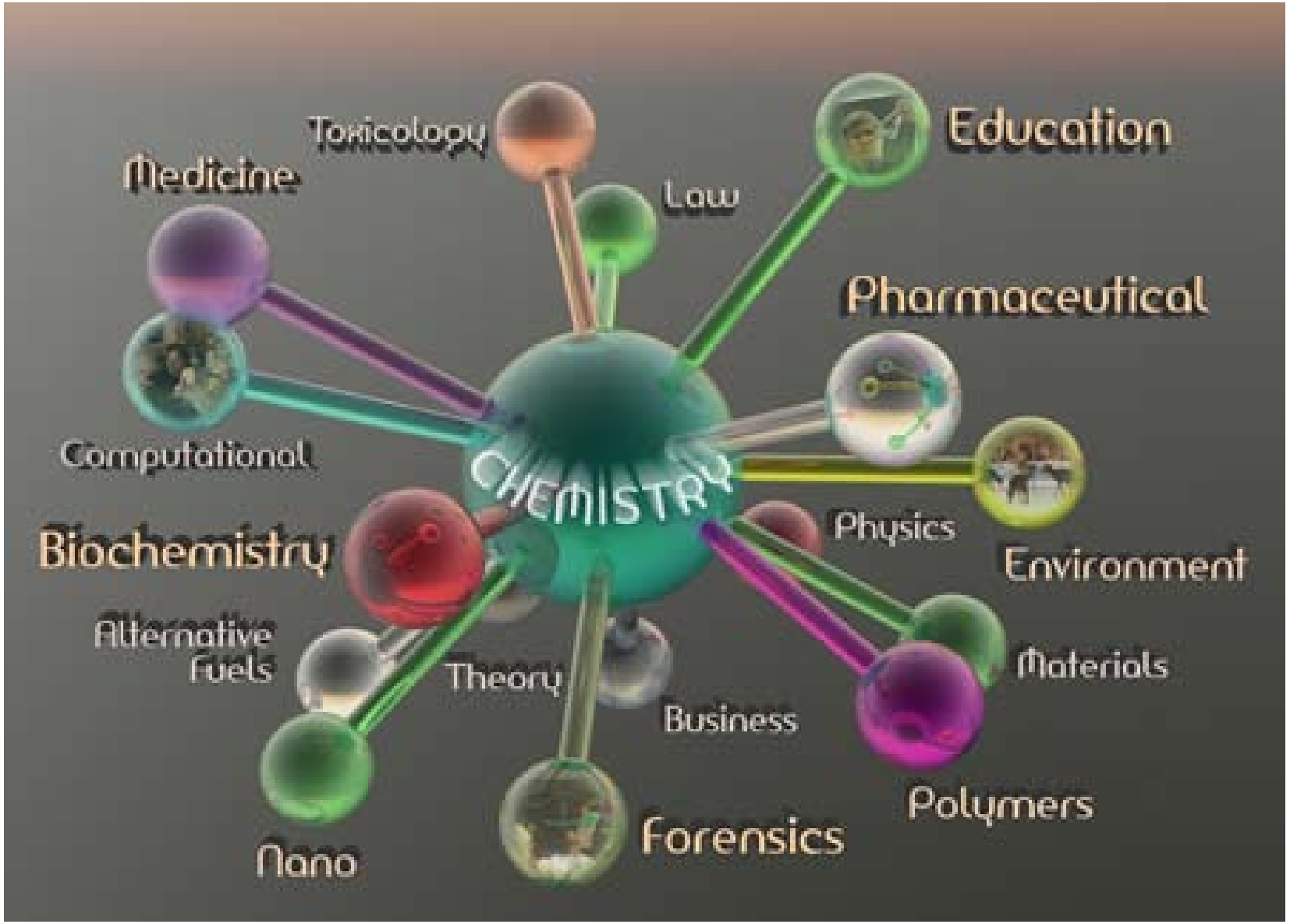


Chemistry is everywhere

Chemistry is everywhere

“Chemistry is often called "the central science" because it connects the other natural sciences such as astronomy, physics, material science, biology, and geology”.

Branches of Chemistry

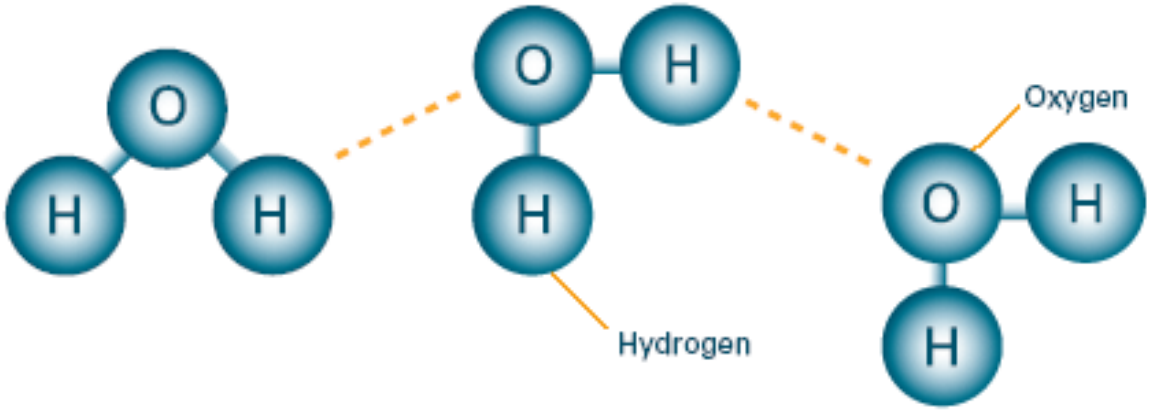


Bonding The Heart of Chemistry

Ionic Bond (Sodium Chloride [table salt])

Covalent Bond (Chlorine Gas)

Hydrogen Bond (Water Molecules)



Invisible ink

- Mix equal parts water and baking soda paintbrush to write a message onto white paper using this solution
- Allow the ink to dry
- paint over the paper with purple grape juice. The message will appear in a different colour.

http://chemistry.about.com/cs/howtos/ht/invisibleink2.htm

Baking soda and grape juice react with each other in an acid-base reaction, producing a colour change in the paper.

http://chemistry.about.com/cs/howtos/ht/invisibleink2.htm

Ice cream in a bag

Combine the sugar, half-n-half, and vanilla in the pint size ziploc bag and seal tightly. Combine the ice and salt (sodium chloride) in the large ziploc bag.

Place the small bag inside of the larger bag and seal. Shake the bag until the mixture turns into ice cream! This will take about 5 minutes.

http://chemistry.about.com/cs/howtos/a/aa020404a.htm

- Ice has to absorb energy in order to melt, i.e. to change from a solid to a liquid.
- When ice is used to cool the ingredients for ice cream, the energy is absorbed from the ingredients and from the outside environment
- When you add salt to the ice, it lowers the freezing point of the ice, so even more energy has to be absorbed from the environment in order for the ice to melt.

http://chemistry.about.com/cs/howtos/a/aa020404a.htm

- This makes the ice colder than it was before.
- Use of larger crystals take more time to dissolve in the water around the ice, which allows for even cooling of the ice cream.
- Salt used should be ionic salt. Sugar cannot be used instead of salt

http://chemistry.about.com/cs/howtos/a/aa020404a.htm

Why apple turn Brown when peeled ?

iron-containing chemicals inside apple cells react with oxygen in the air.
The chemical reaction is called "oxidation", and the enzyme that regulates oxidation in apples is called "polyphenol oxidase" (PPO), also known as "tyrosinase".

http://chemistry.about.com/od/chemistryfaqs/f/brownapplefaq.htm & Chemistry for every kid by Janice Vanclave

WAYS TO KEEP YOUR APPLES FROM GOING BROWN

- vitamin C prevents it from going brown.
- Remove the air from your apples.

This is why vacuum-packed canned foods stay fresh so long.

- Remove water from your apples

(called"dehydration"). Polyphenol oxidase and just about everything else that can spoil food needs water to work.

- Use clean, high-quality cooking utensils. Iron salts found on steel cooking utensils corroded by organic acids can act as potent catalysts to oxidation by producing per-oxides and super-oxides.
- Cook your apples. Heat "denatures" (changes & weakens) polyphenol oxidase.

http://chemistry.about.com/od/chemistryfaqs/f/brownapplefaq.htm & Chemistry for every kid by Janice Vanclave

OR Eat your apples quickly...before they have time to go brown!

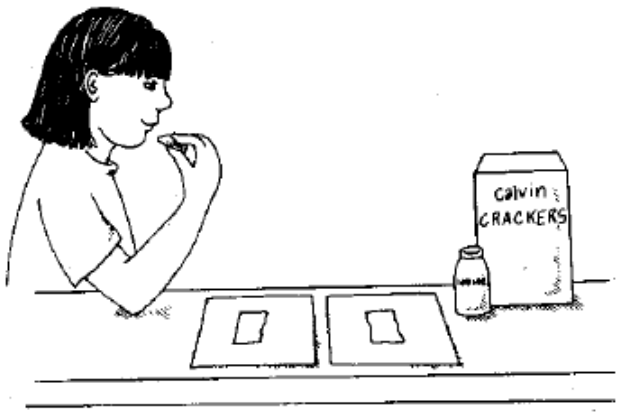
Chemical Reaction in mouth

- Cut 2 small pieces of white bread
- Place one piece in mouth and

  chew it 30 times it will become

  very mushy mix as much saliva

  as possible with bread



- Spit the mushy bread and saliva mixture onto a piece of waxed paper
- Place second dry piece of bread on separate piece of waxed paper .
- Add 4 drops of iodine to both bread pieces

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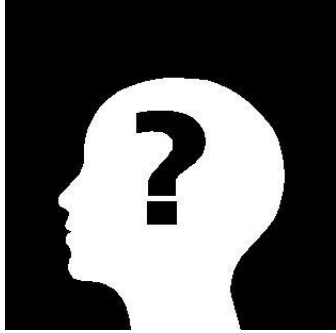
Result: The unchewed bread turns a dark blue-purple. The bread saliva mixture does not turn dark.



The starch in the bread combines with iodine to form an iodine-starch molecule. These molecules are blue-purple in color. Chewing the bread mixes it with saliva. The saliva chemically changes the large starch molecule to smaller sugar molecules. Sugar does not react with iodine, thus no specific color change

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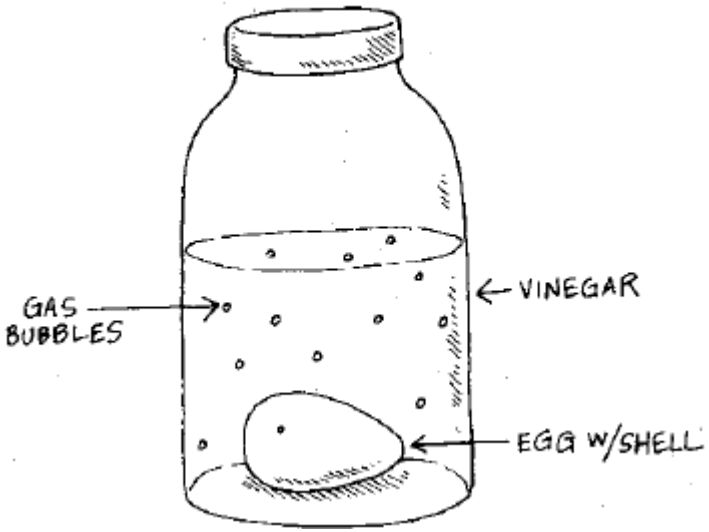
Naked egg



- Place the whole raw egg into the glass jar. Do not crack the egg.
- Cover egg with the clear vinegar.
- Close the lid on the jar.
- Observe immediately and periodically for 24 hours

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Result: Bubbles start forming on the surface of the egg shell immediately and increase in number with time. After 24 hours the shell will be gone, and portion of it may be floating on the surface of vinegar. The egg remains intact because of the thin membrane and yalk can be seen through it

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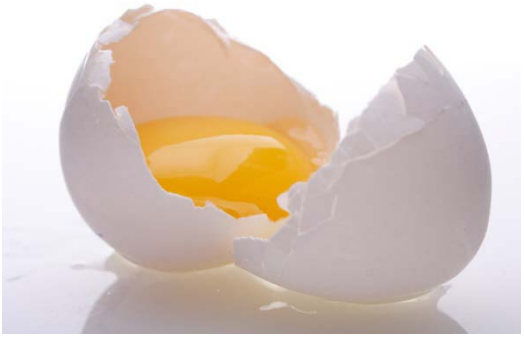

Vinegar's chemical name is acetic acid.

Egg shells are made of calcium carbonate.

The reaction between acetic acid and calcium carbonate causes the egg shell to disappear and carbon dioxide bubble to form.

Erupting Volcano

- Place the soda bottle in pan.
- Shape moist dirt around the bottle to form a mountain. Do not cover the bottle's mouth and do not get dirt inside the bottle.
- Pour 1 tablespoon of baking soda into the bottle
- Colour 1 cup of vinegar with the red food colouring and pour the liquid into the bottle

Result : Red foam sprays out of the top and down the mountain dirt

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The baking soda reacts with the vinegar producing carbon dioxide gas. The gas builds up enough pressure to force the liquid out the top of bottle. The mixture of the gas and the liquid produces the foam

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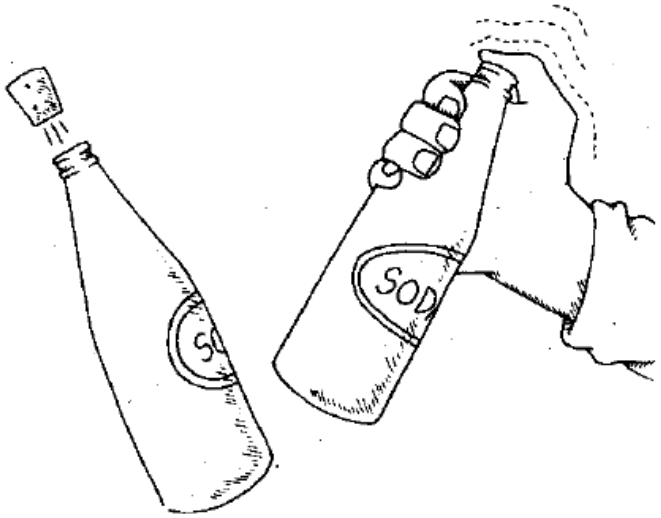
Pop Cork



- Pour ½ package of yeast into soda bottle.
- Fill the bottle one-half full with warm water.
- Add 1 teaspoon of sugar
- Place a thumb over a bottle's mouth and shake the bottle vigorously to mix the contents.
- Cover the sides of cork with petroleum jelly.
- Loosely stopper the bottle with cork.
- Place bottle on the ground

Result: After a few minutes the cork pops out of the bottle

Yeast contains tiny plants that use sugar and oxygen to produce energy. As this energy is produced carbon dioxide is also formed. As the amount of carbon dioxide gas increases inside the close bottle, the pressure of the gas builds. When enough gas is formed , the cork will be pushed out with enough force to produce a popping noise.

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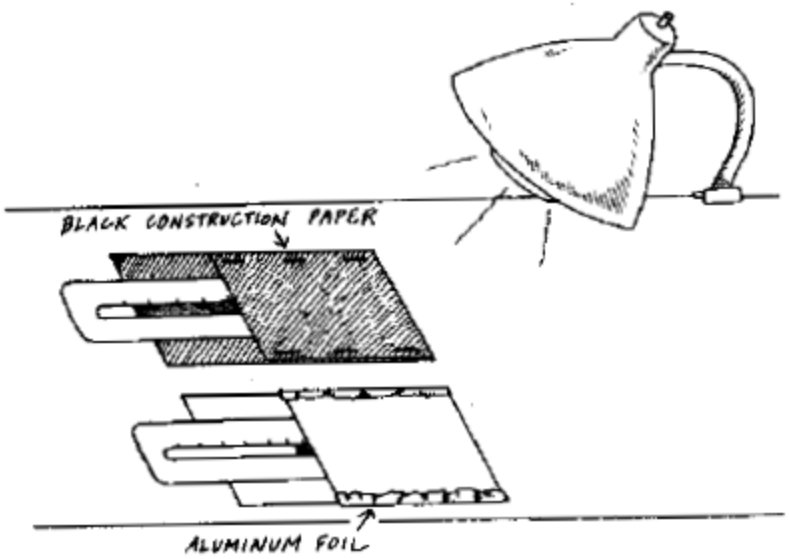
Different colors from flame

When excited by a flame, each element emits light of specific wavelengths that can be used to identify it. The characteristic colors are generated by salts of various elements—red from strontium and green from copper

http://www.physlink.com/Education/askExperts/ae569.cfm

Radiation

- Fold the black construction paper over the thermometer as shown and staple the sides
- Fold a piece of aluminum foil over the second thermometer. Fold the sides of foil over the foil as shown to secure them.



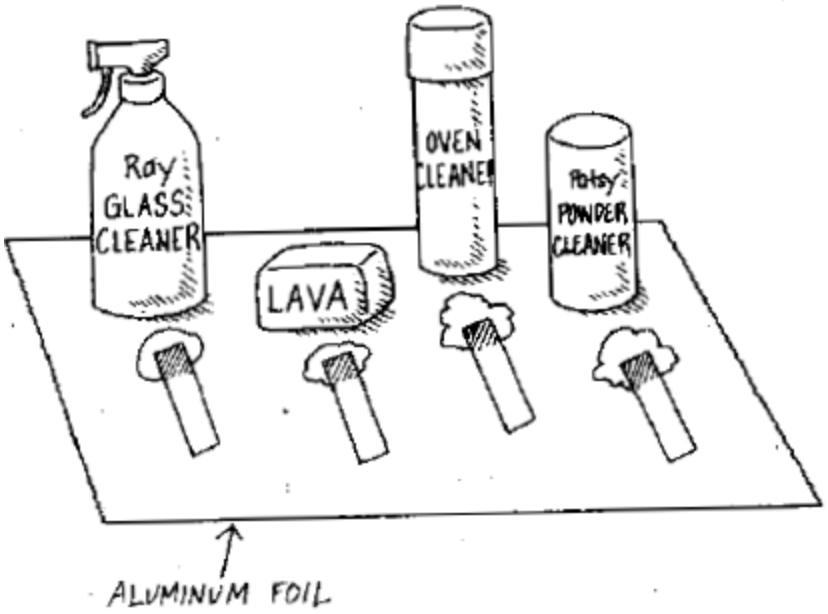
- Record the temperature on both thermometers.
- Place the light source about one foot above the pouches with the thermometers.
- Focus the light on it and observe the temperature readings for 10 minutes

Result: The temperature reading is higher on the thermometer in the black pouch.

Black object absorb all of light waves. Since none of the waves of light are reflected back to the viewer the object looks black. This absorption of waves of energy causes the object's temperature to rise. The aluminum foil does not absorb very many of light waves, thus, its temperature is lower. Spring and summer cloths are usually light in color, so the wearer stays cooler.

Basic Cleaners

- Lay the sheet of aluminum foil on a table.
- Place ½ teaspoon of each of the four cleaners on the aluminum foil. Space them so that they do not touch.



- Dip the end of one turmeric strip in the water. Lay the wet end on one of the testing materials.
- Continue to wet the turmeric strip until one is placed on top of each of the four material to be tested.

Result: All four of the strips turn red where they touch the materials.

Many cleaners are basic. This is because bases combine with grease to form soap. The cleanser reacts with the unwanted grease and the soap that is formed is washed away.

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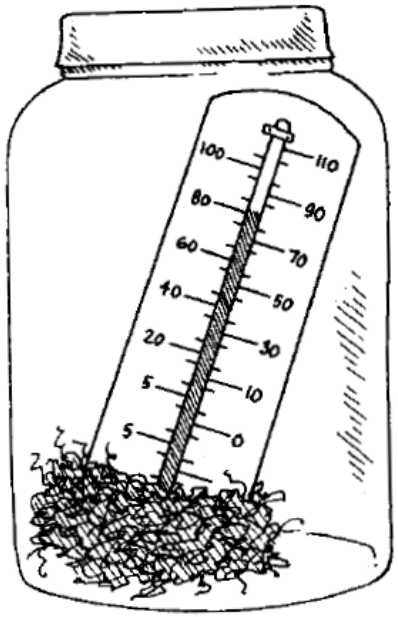
Chemical Heating



- Place the thermometer inside the jar and close the lid. Record the temperature after five minute.
- Soak one-half of the steel wool pad in vinegar for one or two minutes.
- Squeeze out any excess liquid from the steel wool and wrap it around the bulb of the thermometer.
- Place the thermometer and the steel wool inside the jar. Close the lid.
- Record the temperature after five minutes.

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Result: The temperature rises.

The vinegar removes any protective coating from the steel wool, allowing the iron in the steel to rust. Rusting is a slow combination of iron with oxygen, and heat energy is always released. The heat released by the rusting of the iron causes the liquid in the thermometer to expand and rise in the thermometer tube.

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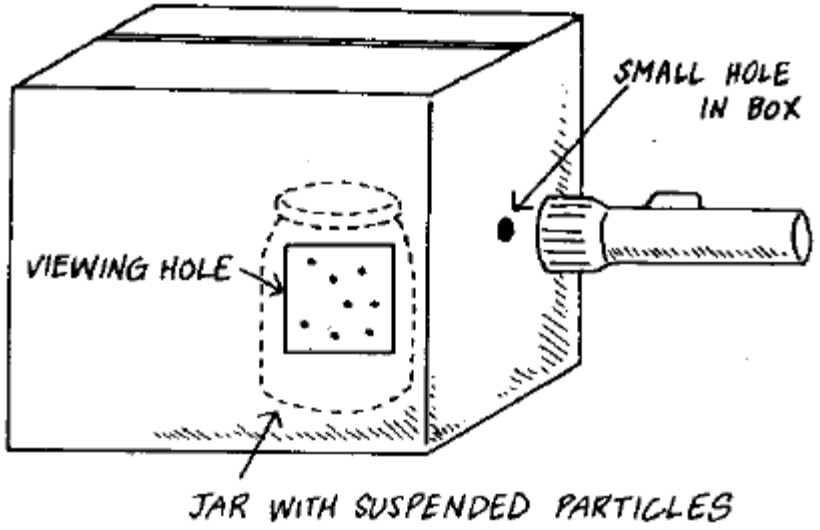
Tyndall Effect



- Turn the cardboard box upside down.
- Use the point of a pencil to make a small hole in the end of the box.
- The height of the hole should be one-half the height of the glass being used.

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- Cut a one-inch square viewing hole in the front of the box. The hole must be about three inches from the corner of the box and as high as the small round hole on the side
- Fill the glass three-quarter full with water
- Add 1 teaspoon of flour to one of the glasses with water and stir.

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- Place the glass containing water and flour under the box. Position the glass so that it is in front of the viewing hole.
- Hold the flash light near the small hole.
- Put the glass containing only water under the box.
- Shine the light through the hole and observe the effect that water has on the light rays.

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Result: The mixture of flour and water looked cloudy. Tiny particle of flour could be seen floating in the water. The glass of water had no effect on the light rays, they passed through the water unchanged

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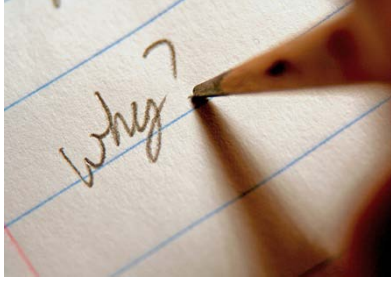

Flour and water form a suspension.

A suspension has tiny particles in the liquid.

The particles stay suspended until gravity pulls them down. The suspended particles stop some of the light rays. Light hits the bits of flour floating in the water and is reflected. Reflect means to bounce back. There is nothing in the water to reflect the light. Reflection of light by suspended particle is called the Tyndall Effect, named after the British scientist, John Tyndall.

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Computational Chemistry

- A branch of chemistry wherein the principles of Physics are applied to understand structure and properties of chemical matter. It is highly useful in situations where direct access to experimental study is not feasible. It also provides useful understanding and interpretation of experimental results.
- Computational chemistry has infiltrated just about every subdiscipline of chemistry. Once-theory-shy experimentalists now routinely include calculations in their experimental papers

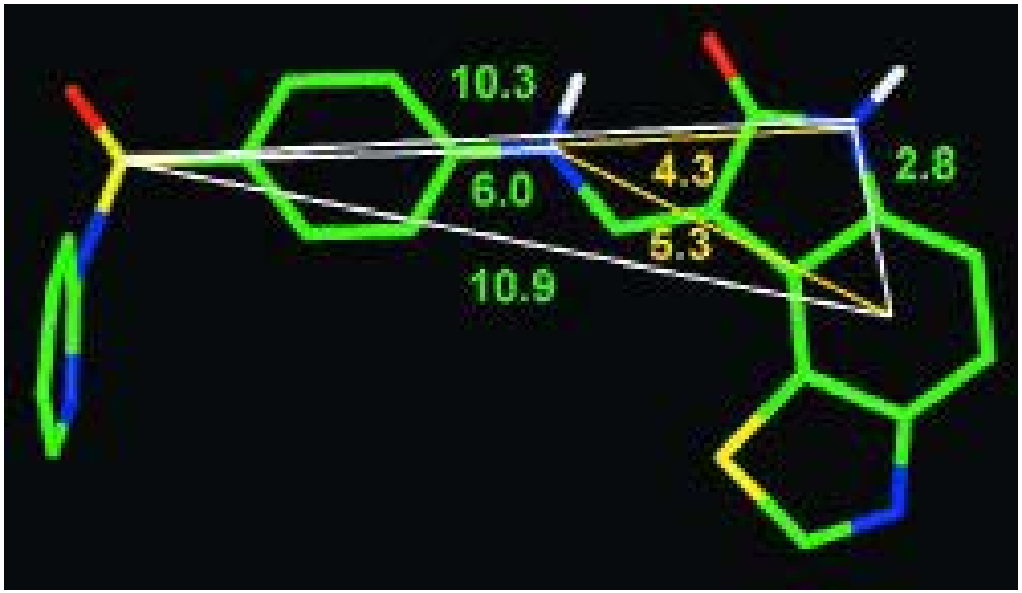
Computational Chemistry

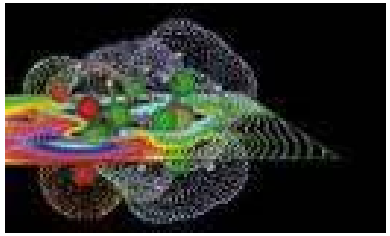
- Using theory, computers and fast algorithms to solve complex equations from theory
- Predict in computers structure and properties of molecules
- Predict reactions between molecules (if the reaction takes place and how fast ??)
- Dynamics of evolution
- Modeling new materials
- Biological activity

Computers in Chemistry

- A computer server harnesses the formidable collective computing power of hundreds of networked desktop computers that for the most part lie idle. While someone's out to lunch or in a meeting, his or her computer can join the "collective" to help crunch huge databases or solve complex equations.
- Problems: Materials – Search for New Materials, Biology- Activity, New molecules and drugs
- Tools: Theories- Quantum/ semi-classical/ Classical, Algorithms, Powerful computers (Servers, distributed , Grid)

- **Pharmacophoric points in oxindole B, found by SCAMPI on a virtual cluster.**
  COURTESY OF C. KEEFER





Assembly of lipoprotein particles revealed by coarse-grained molecular dynamics simulations

Amy Y. Shih, Peter L. Freddolino, Anton Arkhipov , Klaus Schulten

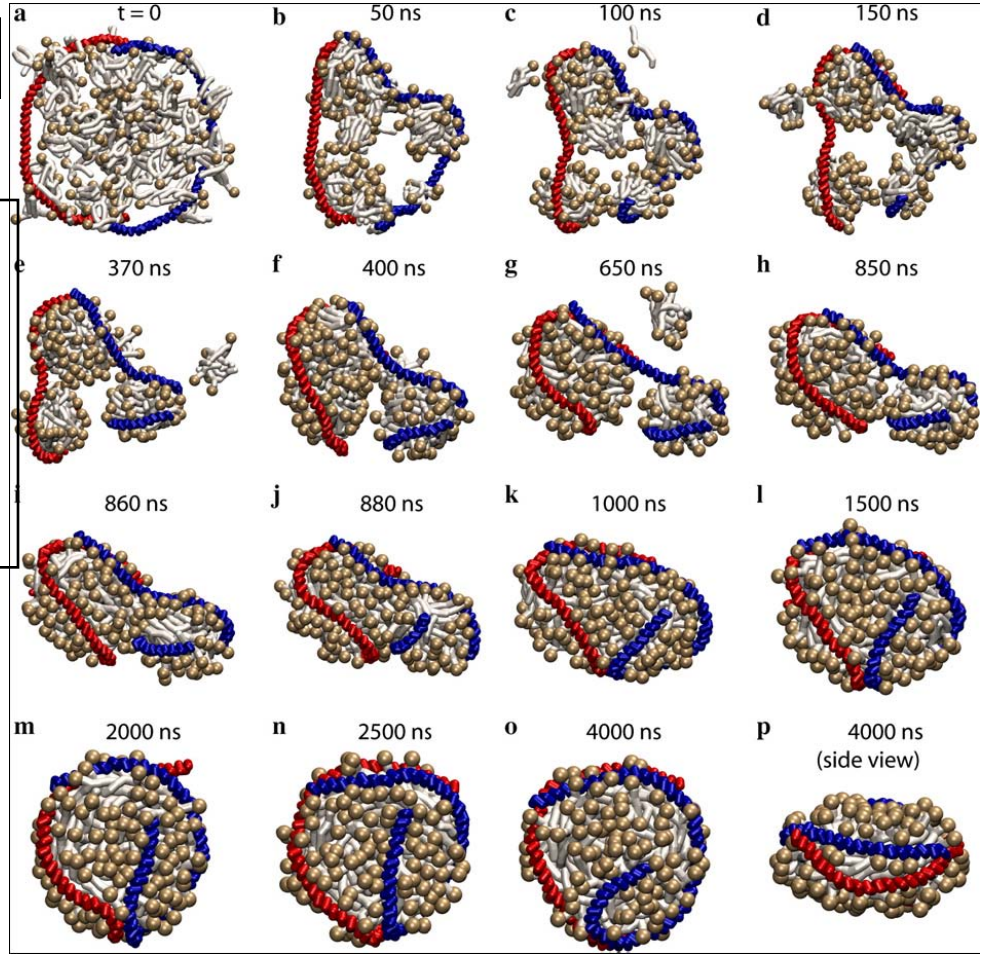
Journal of Structural Biology 157 (2007) 579–592

Good Cholesterol

36 018 CG beads
2 half-circle proteins
160 DPPC lipids

Represents about
500 000 atoms??

25fs time step



Theoretical and Computational chemistry at NCL

Areas of work and Expertise:

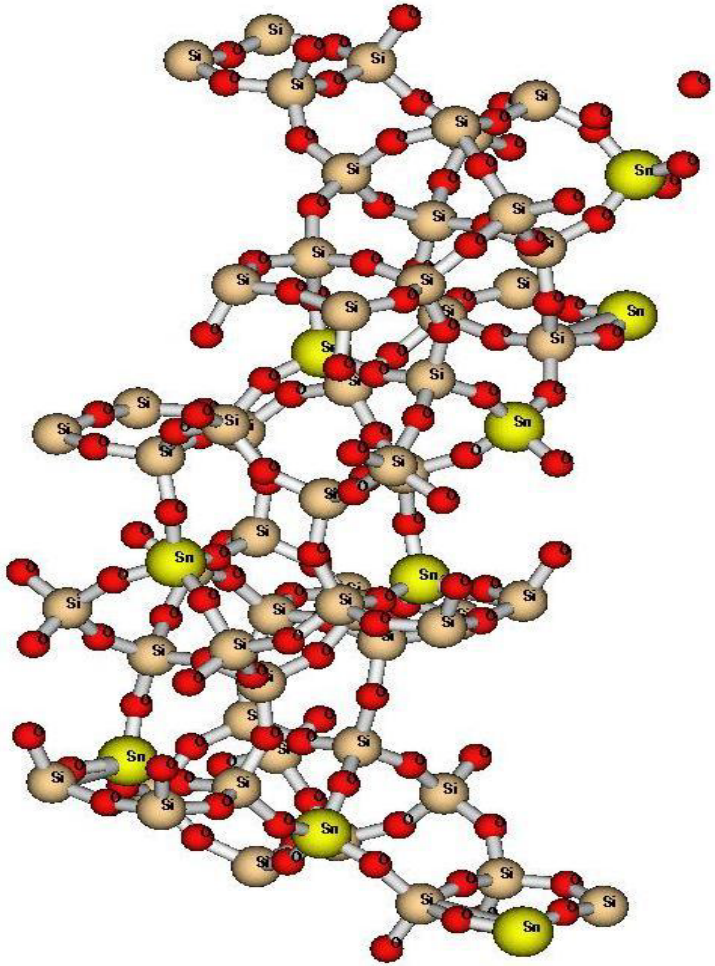
- Electronic structure of molecules
- Structure and spectra of model confined systems
- New descriptors to address reactivity of molecules
- Development of many-body coupled-cluster based methods for molecular properties
- Development of non-iterative approximation of density functional response for large systems
- Principle of minimum magnetizability
- Structural, electronic and bonding properties of Sn-beta zeolite
- Inter-cluster reactivity of Metallo-aromatic and anti-aromatic compounds and their applications in Molecular Electronics
- Metals and doped metals as hydrogen storage materials

Theoretical study of structural and electronic properties of Sn-substituted beta zeolite

- We have used the periodic DFT approach to study the properties of Sn-BEA zeolite in crystalline phase.

- Each of the 9-active sites in the BEA were substituted by Sn and were optimized using the periodic DFT.

- The cohesive energy and the HOMO-LUMO gap obtained for all the 9 sites showed that the site 2 is the most probable site for the substitution of Sn in BEA.



Shetty, Pal, Kanhere and Goursot, Chemistry: A European Journal,12, 518-523 (2006); Shetty, Kulkarni, Kanhere, Goursot and Pal, J. Phys. Chem B (2008)

Science as a Career

- Science provides basic expertise
- Physics, Chemistry, Mathematics, Biology, Geology etc. provide platform for inter-disciplinary research
- Academic research and teaching
- Research with industrial relevance
- Alternate science career
- Freedom and fulfilment of mind