Exploring Augmented Reality interactions to understand the concept of hybridization in organic chemistry

By

Rubayat Ahmed

Roll no. 216330013

M.Des IxD, 2021-23

Project Guide

Prof. Jayesh S. Pillai

IDC School of Design, IIT Bombay

Approval Sheet

The Interaction Design Project- 2 titled “Exploring Augmented Reality interactions to understand the concept of hybridization in organic chemistry” by Rubayat Ahmed, Roll Number 216330013 is approved in partial fulfillment of the Master in Design Degree in Interaction Design, Indian Institute of Technology Bombay.

Project Guide

Chairperson

External Examiner

Internal Examiner

Declaration

I declare that this written project submission represents my own ideas and work in my own words, and if any idea or work has been included, I have adequately cited and referenced the original source. I also declare that I have adhered to all the principles of academic honesty and integrity and have not misinterpreted, fabricated or falsified any idea/ data/ fact source in my submission.

I understand that any violation of the above will be cause for disciplinary action by the institute and can also evoke panel action from the sources.

Rubayat Ahmed
Roll no. 216330013
M.Des IxD, 2021-23
IDC School of Design, IIT Bombay
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Rubayat Ahmed

Abstract

Spatial ability plays an important role in chemistry learning, as students are required to visualize specific microstructures, but the visualization of chemistry topics is a difficult task for students with traditional methods. Teachers and academicians use various analogies and methods to help students understand the topic. Still topics like Hybridization which is a very abstract concept in itself where multiple atomic orbitals are mixed together to form new hybrid orbitals, students find difficulty in understanding the concept and end up mugging it. This project is focused on how we can visualize the concept of hybridization in a more intuitive manner for students with the help of augmented reality. As augmented reality is becoming more accessible day by day, it's a good opportunity for teachers as well as students to leverage the capabilities of AR for better learning opportunities. Objective of the project is to develop a working prototype through novel design interventions in augmented reality, while exploring different marker based interaction techniques.

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Introduction

Like most of the concepts of chemistry that School students can't relate to at a microscopic level, Hybridization of atomic orbital is also a difficult topic to understand without proper spatial visualization. The theory of hybridization is also one amongst the abstract chemistry topics and difficult for students to grasp and comprehend. Students do not enter a chemistry course with any preconceived notions about hybridization because this concept is not encountered in everyday life. Also existing methods of teaching like 2D drawings, explanatory videos, Ball and stick models are not enough to grasp the concept properly. Most of my classmates, including myself, found it difficult to visualize these concepts when I was in 11th grade. I recall teachers attempting various methods to help us visualize it, but many of my friends were unable to grasp the entire concept and ended up mumbling the notes for the exam. This personal issue became the driving force behind my decision to pursue this project. While thinking about possible solutions, two ideas came to mind. The first was an interactive website where students could interact with 3D models of atoms and orbitals, play with them, and learn from them. The second was to use augmented reality to interactively visualize the topic. The latter was selected because it is more immersive and engaging than a website giving much more control in terms of both tangible and digital interactions. Also a website is also always dependent on an active internet connection, whereas AR applications do not and can run on any Android device.

Target Audience

The topic Hybridization is taught in chapter 4 (Chemical Bonding) of the first part of the chemistry NCERT class XI textbook. The topic is also extensively used in organic chemistry which is taught in Class XII. So the primary audience for whom I would be developing the solution are students in grades XI and XII. This can also be used by students who have completed their secondary education and are preparing for engineering and medical entrance exams.

Secondary users could include teachers who want to use it as a supporting tool in the classroom. However, the solution will be designed with keeping the students in mind.

Scope

The project scope is to design a better way to learn the Orbital Hybridization topic conceptually and remove any misconceptions regarding the topic through a holistic instructional design approach and Augmented Reality based immersive interactions. The outcomes of the project will be a supporting material that students can use along with their regular chemistry courses. A booklet with all the study material and instructions along with an android application to facilitate the AR activities are what I aimed to deliver at the end.

Background

The popular perception of an atom as a miniature solar system (as shown in figure 1), with electrons behaving like planets orbiting a star (the nucleus), works in some cases, but it is not how an atom actually behaves. The problem with this approach to atoms is that electrons can never be precisely located and must instead be conceived of as existing in the space available to them. It is due to electrons' dual nature, which is both wave and particle nature. To make things easier, only the particle nature of electrons is highlighted in school textbooks.

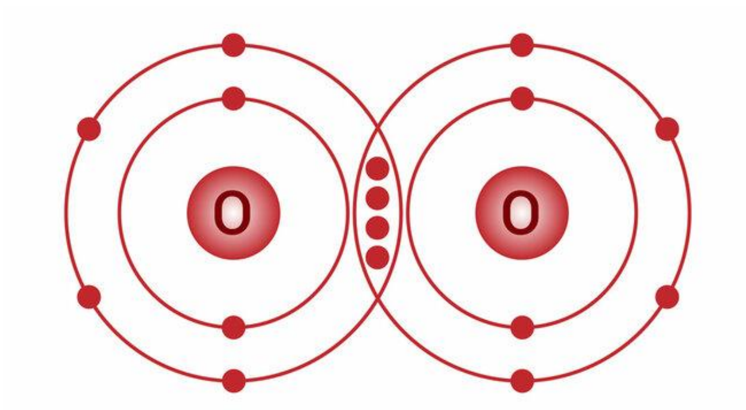

Fig 1. Schematic representation of atoms

To understand concepts like hybridization, however, one must first understand the actual characteristics of an atom and its elements.

Definition of Orbitals

We have to think of electrons in atoms (and in molecules) as having a probability of being in a certain place at a certain time, and the sum of all these probabilities gives a smeared out picture of the electron's habits, a bit like blurred pictures of the vibrating strings(Fig. 2).

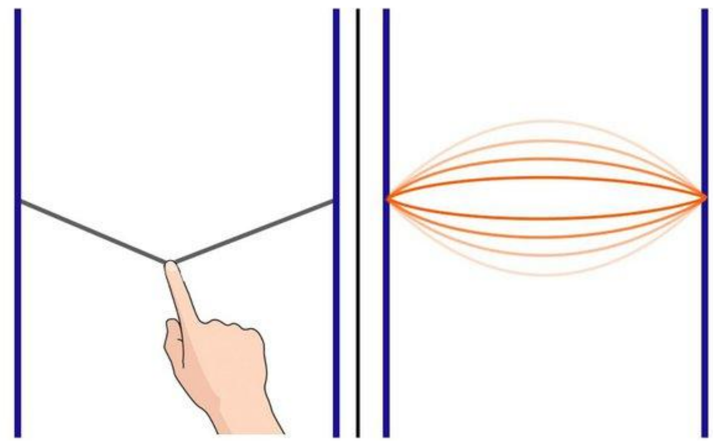

Fig 2. Blurred illustration of a vibrating strings

Consider a stretch string or guitar string that is tied at both ends. If you hit it or pluck it, it will vibrate in the manner depicted in the diagram above(Fig. 2). We could also represent a 'blurred' image of all the locations where the string could be found as it vibrates. Similarly the 3 dimensional space around the nucleus where an electron can vibrate are known as orbitals, or atomic orbitals. There are 4 atomic orbitals s, p, d, and f. We will cover only s and p orbitals in this course as these orbitals are mostly used and taught in school.

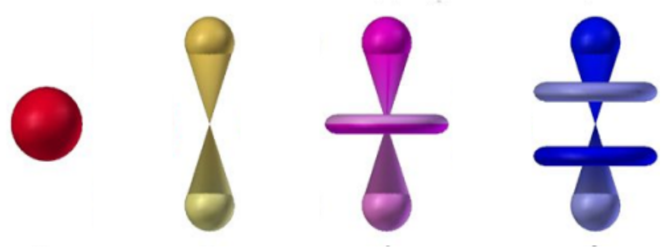

Fig 3. Schematic representation of all the four orbitals(s, p, d and F)

S Orbital

The smeared-outp image of the simple atomic orbital resembles the image below (Fig. 4). Shading is used to indicate the likelihood of finding an electron at any given point. Drawing a line (in reality a three-dimensional surface) around the space where an electron vibrates is a more convenient way to represent an orbital. But it misleads many students to think of it as a path or a strict boundary inside where an electron resides.

Fig 4. Various ways of representing s orbital

This simplest possible orbital, the fundamental orbital of the H atom is spherical, and is known as a 1s orbital. Other orbitals have different shapes like p has a dumbbell kind of shape, Each of these orbitals can have maximum 2 and minimum 0 electrons.

Node

Previously shown vibration is not the only way the string can vibrate. An alternative possibility is shown below(Fig. 5), where not only are the ends of the string stationary, but so is the point known as a 'node' right in the middle. On the string the node was the point where no motion was observed.

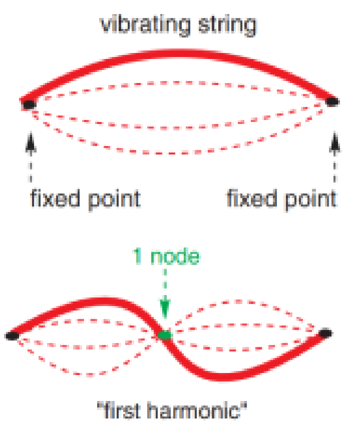

Fig 5. Various ways of representing s orbital

Similarly in an atom, a node is a point where the electron can never be found, a void separating the two parts of the orbital.

Phase

As seen in the figure 5, the left-hand half of the string moves upwards while the right-hand half moves downwards, the two halves of the string are out of phase with one another, and there is a change of phase at the node. The same is true for orbitals also. The 1s orbital, which doesn't have any node to divide the orbital into two parts, can exist in any one of the phases either positive or negative.

Overlapping of s orbital

Just as atoms add together to give molecules, we can add together the wavefunctions of atomic orbitals to give molecular orbitals, which tell us where electrons are, and how much energy they have, in molecules. As atomic orbitals are wavefunctions, they can be combined in the same way that waves combine. Let's look at how waves combine or overlap.

1. **In phase overlapping**: When two waves of similar phase combine they add up to each other and produce a single wave of higher amplitude. It is called constructive overlapping.(Fig. 6)

Fig 6. In phase overlapping

Similarly two in-phase S orbitals overlap with each other to form a new orbital. The diagram of the orbital shows that the electrons would spend most of their time in between the two atomic nuclei. Being negatively charged, the electrons will exert an attractive force on each of the nuclei, and would hold them together. We have a chemical bond! For this reason the in-phase molecular orbital is called a bonding orbital. The two electrons between the two nuclei in the bonding molecular orbital hold the molecule together — **they are the chemical bond.**

2. **Out of phase overlap**: But if waves of opposite phase combine they produce lower amplitude waves subtracting each other's amplitude. It is called destructive overlapping.(Fig. 7)

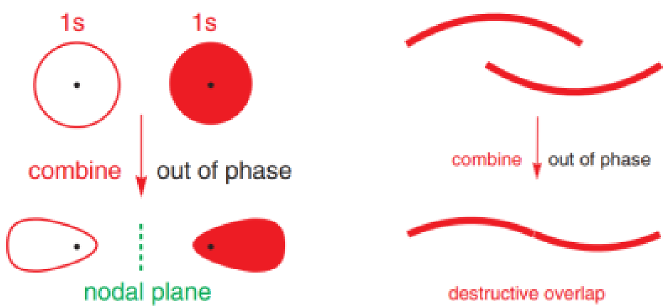

Fig 7. Out of phase overlapping

The out-of-phase molecular orbital offers no such attractive possibility. These electrons are mainly to be found anywhere but between the two nuclei, where there is a node. The exposed positively charged nuclei repel each other, and that is why this orbital is known as an antibonding molecular orbital.

P Orbital

The node where there is no chance of finding an electron can alternatively be a plane. This alternative arrangement for an orbital with a single planar node gives us a new type of orbital, the ‘p’ orbital. A ‘p’ orbital looks something like the picture on the left below(Fig. 8), in ‘smeared out’ form. A nodal plane, such as that in the 2p orbitals, divides the orbital into two parts with different phases, one where the phase is positive and one where it is negative

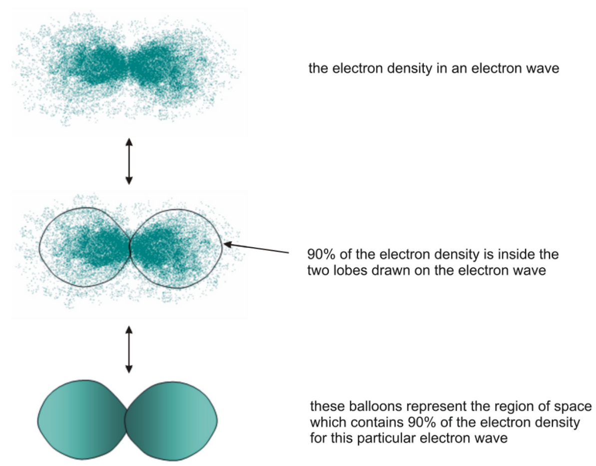

Fig 8. Out of phase overlapping

Directionality of P orbital

Unlike the 1s or 2s orbitals, the p orbital is directional. It points along an axis, and in three dimensions there are three possible orientations for the axis, each of which gives rise to a new p orbital (which we can call px, py and pz). All these three orbitals stay together as seen in the figure 9.

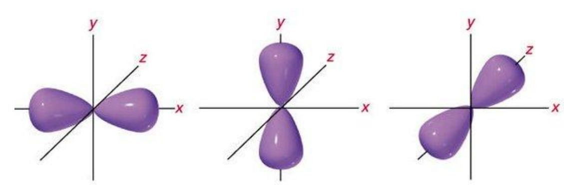

Fig 9. Px, Py, Pz orbitals

Overlapping of p orbital

As we learnt there are two types of overlapping, in phase or out of phase, P orbitals also exhibit similar overlapping. But there is a new kind of overlapping apart from the head-on overlapping that P orbitals can do because of their directional properties, which is sidewise overlapping. The bonding orbital formed by head-on overlapping is called Sigma bond while the bonds formed by sidewise overlapping is called Pi bonds.

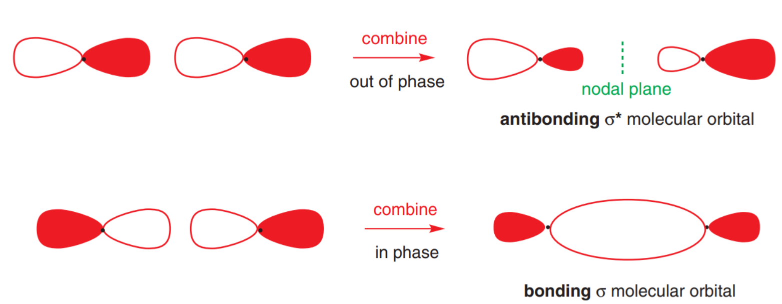

Fig 10. Head-on overlapping of P orbitals

Sigma and Pi Bond

Let's consider the end-on overlap first. If we combine the orbitals in phase, what we get is a nice rich area of electron density between the nuclei, so overall filling this orbital with electrons would lead to an attraction between the atoms and a bond would result, which is known as sigma (σ) bond.(Second diagram of Fig. 10)

Similarly if we arrange them side-by-side parallelly in phase we get a space where electron can present mutually, forming Pi (π) bonds, and you'll notice that electron density in these bonds does not lie directly between the two nuclei but rather to either side of the line joining them causing less stronger bond compared to Sigma bonds.

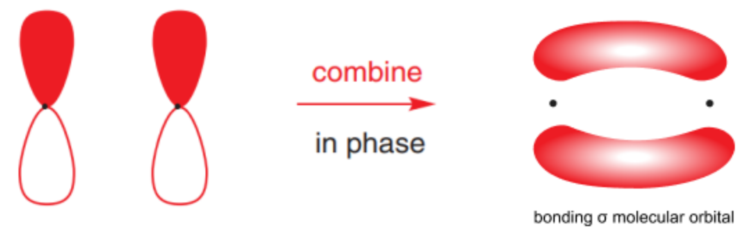

Fig 11. Side by side overlapping of P orbitals

Atomic Orbital Hybridization and its significance

The process of combining two atomic orbitals to create a new type of hybridized orbitals is known as hybridization. This intermixing frequently results in the formation of hybrid orbitals with completely different energies, shapes, and so on.

Hybridization holds a very important role throughout the entire subject, as it is considered as one of the main theories explaining how atoms share electrons and form molecules. It is taught in chapter 4 (Chemical Bonding) of the first part of the chemistry textbook of class XI (NCERT). Also in the later part, the reference of it keeps coming mainly in coordination compounds and organic chemistry.

To understand the importance of this theory we must have some basic knowledge of the previous theories based upon which it emerges. Which are as follows…

The valence shell electron pair repulsion (VSEPR) theory : This theory is used to predict 3-D molecular geometry based on the number of valence shell electron bond pairs among the atoms in a molecule or ion. It is based on the premise that there is a repulsion between the pairs of valence electrons in all atoms, and the atoms will always tend to arrange themselves in a manner in which this electron pair repulsion is minimalized. This arrangement of the atom determines the geometry of the resulting molecule.
Limitations of the theory :

1. This theory fails to explain isoelectronic species (i.e. elements having the same number of electrons). The species may vary in shapes despite having the same number of electrons
2. The VSEPR theory does not shed any light on the compounds of transition metals.

Valence Bond Theory : Similarly the VBT theory gives the geometry of simple molecules but theoretically, it does not explain them and also it has limited applications. This theory focuses on the concepts of electronic configuration, atomic orbitals (and their overlapping), and the **hybridization** of these atomic orbitals. Chemical bonds are formed from the overlapping of atomic orbitals wherein the electrons are localized in the corresponding bond region. The valence bond theory also goes on to explain the electronic structure of the molecules formed by this overlapping of atomic orbitals.

Hybridization explains why some molecules have specific structure and geometry that VBT theory predicts but cannot explain. It is recommended to learn hybridization in order to understand VBT, which has further applications in the majority of chemistry topics..

Importance in Organic Chemistry

Carbon's tetravalency allows it to form valuable and useful compounds such as diamond and graphite. Because of its valency of four, it can form bonds with four other atoms. Carbon can form c compounds with oxygen, hydrogen, sulfur, chlorine, and many other elements due to this property. The bonds formed by carbon are extremely strong, making the resulting compound extremely stable. The concept underlying this entire phenomenon is hybridization only.

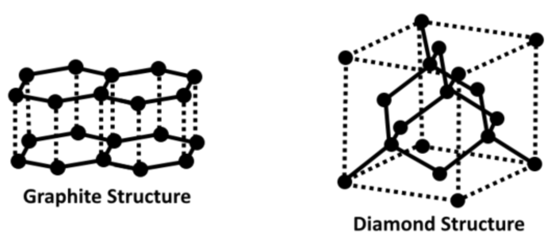

Fig 12. Specific structure of graphite and diamond

Key Features of Hybridization

1. Atomic orbitals with equal energies undergo hybridization.
2. The number of hybrid orbitals formed is equal to the number of atomic orbitals mixing.
3. It is not necessary that all the half-filled orbitals must participate in hybridization. Even completely filled orbitals with slightly different energies can also participate.
4. Hybridization happens only during the bond formation and not in an isolated gaseous atom.
5. The shape of the molecule can be predicted if the hybridization of the molecule is known
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7. The shape of the molecule can be predicted if the hybridization of the molecule is known.

Types of Hybridization

Based on the types of orbitals involved in mixing, the hybridization can be classified as sp3, sp2, sp, sp3d, sp3d2, sp3d3.

sp Hybridization

The hybridization in which only one s orbital and one p orbital involve the same atom, is called sp hybridization. These two orbitals hybridize and form two new sp hybridized orbital of same properties, which take a linear structure forming a 180 degree bond angle.

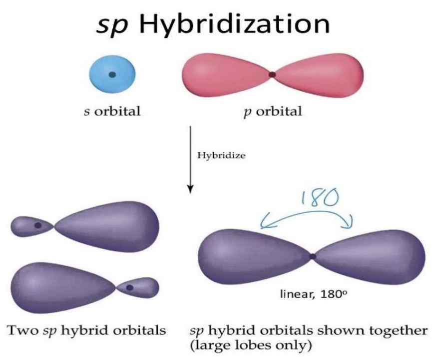


Fig 13. Sp hybridization

sp2 Hybridization

The mixing of one s and two p orbital of the same atom to form three new hybrid orbitals is called sp2 hybridization. All these three hybrid orbitals have equal energies, maximum symmetry and definite orientation in space. The geometry of sp2 hybridized orbitals are triangular bipolar,

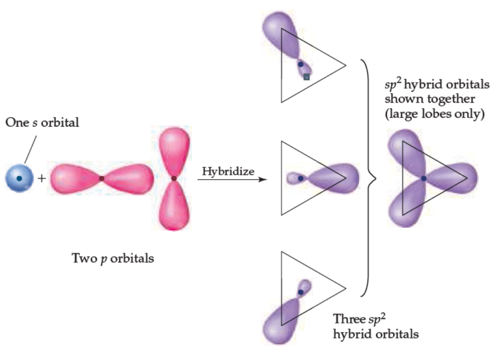


Fig 14. Sp2 hybridization

sp3 Hybridization

The process of Hybridization in which one s and three p orbitals of the same element involves mixing and recasting and forms a new hybrid orbital of same energy, symmetry, and definite orientation in space is called sp3 hybridization. The formation of methane molecules is the example. The geometry of these hybrid orbitals in 3D space is tetrahedron. That is the reason behind the tetrahedral structure of Methane(CH4).

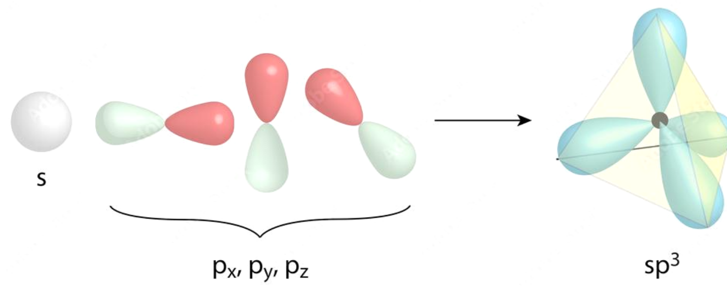
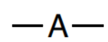
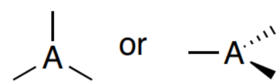
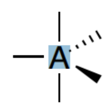
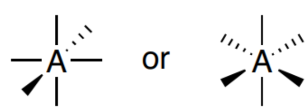


Fig 15. Sp3 hybridization

The Complete Table of Hybridization and Geometry

Number of Electron Domains	Hybrid-ization	Electron-Pair Geometry	Line, Dash, and Wedge Perspective Representation of the Electron-Pair Geometry	Number of Lone Pairs	Molecular Geometry	Bond Angles	Polar? (***)
2	sp (two sp hybrid orbitals) (2 unhybridized p orbitals are available for π bonding)	Linear		0	Linear	180°	No
3	sp^2 (three sp^2 hybrid orbitals) (1 unhybridized p orbital is available for π bonding)	Trigonal Planar		0	Trigonal Planar	120°	No
				1	Bent	< 120°	Yes
4	sp^3 (four sp^3 hybrid orbitals) (0 unhybridized p orbitals are leftover; no π bonding)	Tetrahedral		0	Tetrahedral	109.5°	No
				1	Trigonal Pyramidal	< 109.5°	Yes
				2	Bent	< 109.5°	Yes
5	sp^3d (five sp^3d hybrid orbitals) (0 unhybridized p orbitals are leftover; no π bonding)	Trigonal Bipyramidal	 Note: Contains Axial and Equatorial Positions. Lone pairs (if any) go in Equatorial Positions	0	Trigonal Bipyramidal	90° and 120°	No
				1	See-Saw	< 90° and < 120°	Yes
				2	T-Shaped	< 90°	Yes
				3	Linear	180°	No
6	sp^3d^2 (six sp^3d^2 hybrid orbitals) (0 unhybridized p orbitals are leftover; no π bonding)	Octahedral		0	Octahedral	90°	No
				1	Square Pyramidal	< 90°	Yes
				2	Square Planar	90°	No

Number of Electron Domains (or "Number of electron pairs") = (Number of Other Atoms Something is Bonded To) + (Number of Lone Pairs)

Fig 16. Hybridization details (Image Source : https://canvas.harvard.edu/)

Current methods

Methods	Description	Advantage	Disadvantage
2D illustrations	The most commonly used method in school textbooks.	• Accessible to all students • Flexibility of demonstrating anything	• Unable to visualize spatially. • Can't see the interactive process.
Ball and Stick Models	Physical models of atoms and molecules, used to demonstrate mostly compound structure.	• Give a physical sense of structure, shape, size. • 360 degree view is possible • Can interact with(limited)	• Very limited interactions. Only bond formation can be done. • Not accessible for all students. • Unaffordable in terms of storing and carrying .
3D animations	Tutorial videos made in 3D, that can be accessed with a phone and internet.	• Give a physical sense of structure, shape, size. • 360 degree view is possible • Can show the process	• Not interactive • No control over the student • Content driven, non exploratory.

Fig 17. Current methods of teaching chemistry in schools (Image Source)

Why Augmented Reality

Augmented reality in education is becoming increasingly popular in classrooms around the world. Educators can use augmented reality (AR) to improve learning outcomes by increasing engagement and interactivity. And that's just to get started. AR even outperforms virtual reality in some ways (VR).

From the available immersive media options I choose to go with augmented reality for a few reasons…

1. In AR, users always have a sense of presence in the real world. It will help students to relate to the concepts as these phenomena are also part of the real world.
2. AR will prevent students to trap them isolated inside the medium which happens in case of VR and other immersive mediums. As AR is 25% virtual and 75% real.
3. AR can be used to increase collaboration among the students by engaging them in team oriented AR Activities.
4. It is more easy and affordable to get access to an AR environment. One just needs a smartphone or tablet. While in the case of VR, One needs special HMDs to access the environment.

Types of AR : there are two main divisions of Augmented reality based applications.

1. Marker-based AR : AR applications that use target images (markers) to position objects in a given space are known as marker-based AR applications. These markers determine where the 3D digital content will be displayed in the user's field of view. Markers were the foundation of early-stage AR technologies.

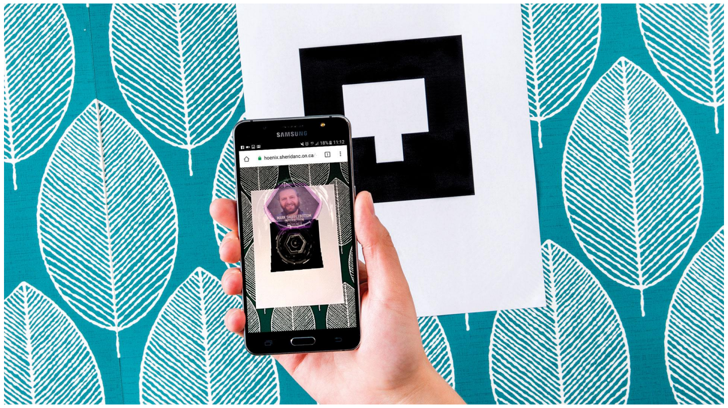


Fig 18. Marker-based augmented reality

2. Markerless AR : In contrast, markerless AR allows virtual 3D objects to be positioned in the real image environment by examining the features present in the data in real time. This type of guidance relies on the hardware of any smartphone, such as the camera, GPS,

or accelerometer, among others, while the augmented reality software does the rest.

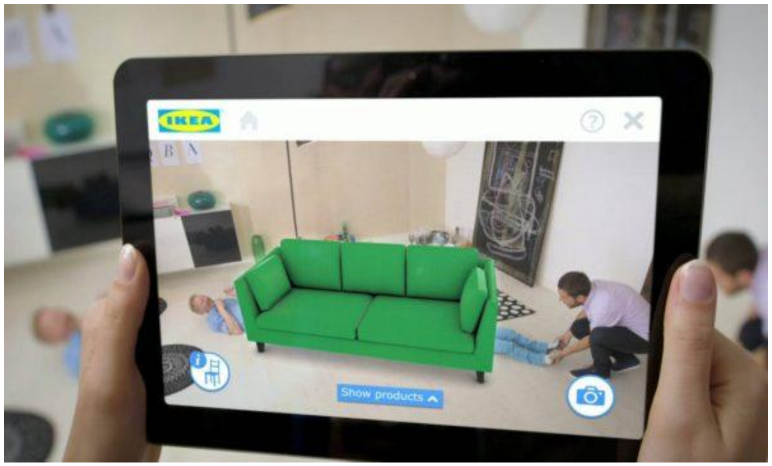


Fig 19. Markerless augmented reality

Primary Research

Though the fact that students face difficulties in visualizing and understanding the concept of hybridization has already been established through various previous research works. I did a quick primary research on how students (specially in Indian Context) perceive this concept and how teachers are helping their students in understanding the concept.

I had done 6 student Interviews (telephonic/video conference) two from class 11, three from coaching and 1 from 12th standard. All of them are from multiple cities across the country and samples through snowball sampling.

The formulated questions are as follows-

1. What is your favorite topic in chemistry? Why?
2. What is the topic that you don’t like at all? Why?
3. Do you get fascinated about atoms, orbitals, and their structure ?
4. What do you think about orbitals(s,p,d)? Do they really exist? Do electrons really move in orbitals? Or are these concepts just analogies?
5. Do you feel difficulty in understanding the VBT, MOT, Orbital Hybridization? If yes can you elaborate?
6. On the scale of 10, what would you rate on your understanding of Hybridization?
7. What is hybridization of orbitals according to you in one line?
8. Could you properly visualize the Hybridization of atomic orbitals during class. If not, what are the difficulties you faced while visualizing the concept?
9. By what methods did the teacher teach hybridization in class? Did she/he used ball and stick models, 3D diagrams, 2D sketches on the blackboard, Videos or just theory?
10. What are your favorite methods to learn these concepts?

11. Any ideas or thoughts which can help me to design a better way of communicating these complex ideas to students?

Interview Insights :

Out of the 6 students interviewed one student who was doing medical coaching came out to be very bright and have almost all the concepts clear. This resulted from the students intense curriculum and deep interest in chemistry. On the other hand Other 5 students gave good insights on the shortcomings of chemistry learning specially in topics like hybridization. Some key insights were -

1. Students mug up the whole topic just to pass the exam
2. Students use shortcuts or formulas to remember hybridisation types in molecules
3. Orbital concept is not clear, 4 out of the 6 students thought orbitals are the path where electron moves
4. Teacher do not use any other method like ball and stick to help student understand the topic
5. Students can't relate to the topics with reality
6. Interests on the topic depends on how the teacher is teaching
7. Students are not aware of the importance of hybridization in context to organic chemistry
8. Take help from youtube to learn more about the topic

Secondary Research

Some secondary research has been conducted in order to identify more critical concepts that students around the world may encounter. The study was based primarily on previous research and articles found on the internet. Many important topics, as expected, were not properly taught or understood by students all over the world. Students have a variety of misconceptions. The following paper logically explains the reasons for these misconceptions.

1. Misconceptions into two categories: experiential and instructional.
2. Many misconceptions are related to theoretical models that require the student to interpret observations in terms of something that cannot be experienced directly.
3. Some misconceptions result from bad instructional experience.
4. Many misconceptions are related to difficulty in following chains of logical inference
5. Students used the notions of orbitals, shells and orbits interchangeably

After analyzing the most common misconceptions that students have regarding this topic we can identify three overall topics

Misconceptions on Atomic orbitals

1. Orbitals are trajectories arranged around the nucleus where electrons rotate.
2. An orbital is a fixed energy level that the electron is found on.
3. An orbital is a place where electrons are arranged to be in order.
4. An orbital is a box that can be full or empty but filled by electrons.
5. An orbital is a line followed by electrons in a determined order.

> **Actual Concept**
>
> The behaviour of an electron in an atom is characterised by a wave function, or orbital, the square of which defines the probability of finding the electron in various regions of space. So an orbital is 3D space around the nucleus where an electron can be found.

Misconceptions on hybridization

1. Hybridization is a process of an atom or molecule to complete the number of their valence electrons to eight.
2. Atoms undergo hybridization because these atoms need electrons to satisfy the octet rule.
3. Hybridization is the transformation of orbitals into energetically equivalent ones.
4. Hybridization is the distribution of electrons to the orbitals equally

> **Actual Concept**
>
> - Hybridization consists of mixing the atomic orbitals of an atom in such a way as to form new hybrid orbitals.
> - Hybridization is a process in which two atomic orbitals having different energy levels form new energetically equivalent hybrid orbitals

Misconceptions on why does hybridization takes place

1. To have a more stable structure.
2. To form a compound in different structures
3. To complete the number of the valence electrons to eight in their last orbits
4. To decrease the energy difference among the orbitals.
5. Because of unoccupied orbitals atoms would like to take electrons.

Actual Concept

- Atoms need half-filled orbitals in order to form bonds. Some atoms need hybridization since they donít have enough half-filled orbitals necessary for bond formation.
- To organise bond formation of atoms and the geometry of the molecules these atoms will undergo hybridization.

Narrowing down the topics

With the knowledge about the topic and understanding over students' problems from various sources of articles and research papers, helped me to further narrow down the scope of the project. The key Insights from the research put lights on some important aspects which need to be taken care while designing the solution. They are -

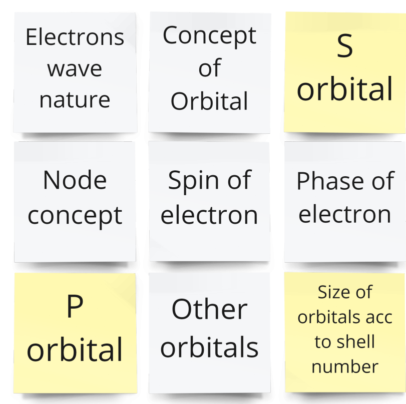
1. Firstly, the concept of Hybridization is not a stand alone topic to be understood, there are many prior concepts and post applications need to be taught to fully understand the topic
2. As these concepts are very abstract and they require the students to have learned the course material meaningfully
3. The atomic orbital concept is one of the most important prerequisite concepts in learning about hybridization
4. Many students were not aware of the importance of hybridization

Considering these points I decided on the following topics to be covered in my design.

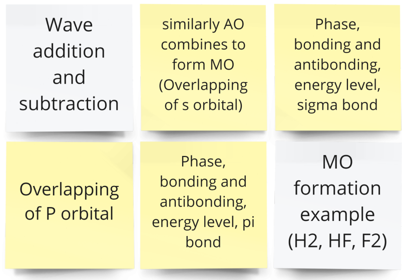
1. Concept of orbital
2. Orbital Overlapping
3. Types of Orbitals
4. Need of hybridization
5. Hybrid orbital formation process
6. Features of hybridization
7. Hybridization in Hydrocarbons
8. More complex examples

These topics can be further dissected into various sub topics. I listed down every such topics and grouped them together in 3 broad topics -

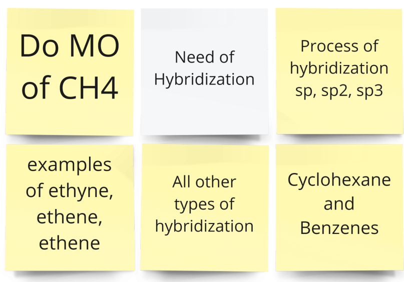
1. Atomic Orbital related topics



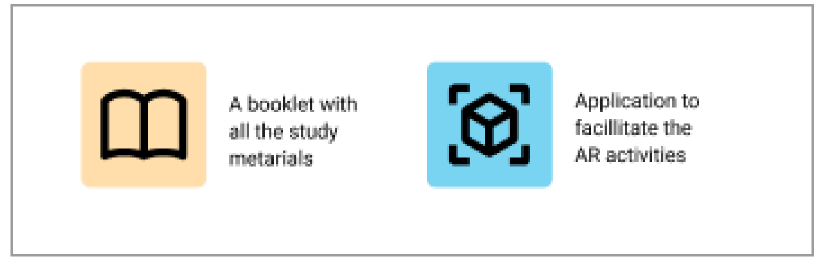
2. Orbital Overlapping related topics



3. Hybridization



Since all of the above-mentioned concepts must be learned sequentially, we will require a common medium to engage students and track their progress. For that purpose, the solution could be either a complete App containing all of the learning material (digital) and AR Activities, or a mixture of a booklet supported by an Application to accommodate the AR activities. I prioritized the second option, which will significantly reduce screen time and give them a feeling of belonging or have something tactile with them. The topics on yellow sticky notes are supposed to be shown in AR, and all the other topics will be covered in the booklet.



Considering the scope of this project, not each of the above concepts can be developed in order to develop a high-fidelity prototype. So , I have reduced the number of concepts to be developed and tested with students without compromising on the core concepts.

I used three levels of learning to filter these core concepts: What, Why, and How. Introductory topics which are crucial to understand Hybridization like orbitals, phase, overlapping are categorized under What. In Why, we try to answer the importance of hybridization through examples and also reasons for hybridization. And at the end, with the help of some implementations the actual process of hybridization and and its types will be demonstrated.

What?	Orbital Overlapping of S and P orbitals Phase, bonding and antibonding, energy level, sigma bond
Why?	Need of Hybridization Build the structure of CH_4 yourself and compare it with the actual structure.
How?	The process of hybridization and its applications in organic chemistry

Design intervention in AR

The capabilities of Augmented Reality allows us to do a lot of things. Leveraging it creatively can bring novel solutions to real life problems. Some creative decisions that I took to implement in my project to develop a better user experience while the students use AR.

1. **Using both plane and cube markers**
   In most of the use cases of marker based AR, plane markers are being used because of its flexibility while usage of cube markers are limited. But Cube markers have a great benefit over plane markers that is 3 degree freedom of rotation. One can rotate it along all the three axes which give users a sense of holding an AR object in their hand. So, I have used cube markers in a few cases to test its usability over the plane markers.

Fig 20. Markers with magnets

2. **Using Magnets for haptic feedback**
   All the topics related to hybridization are associated with attraction and repulsion concepts. Showing it only visually doesn't do much justice when we have tangible markers in use. Tiny magnets strategically attached to the sides of the markers can generate haptic feedback when two orbitals overlap or go away from each other.

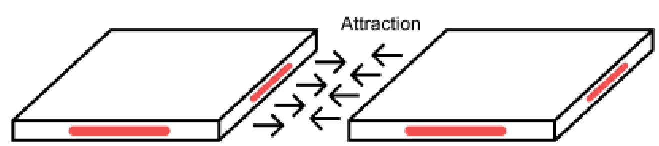


Fig 21. Magnetic attraction and repulsion between markers

3. **Changing scenes according to the sub-topics**
   As mentioned above there will be three main sections or sub topics under Hybridization, which are Orbital overlapping, Need of hybridization and Types of hybridization. So to communicate the order of these topics and the sub-topics multiple scenes are used and students can change between the scenes to learn the topics. This also brings another advantage which is explained in the next point.

4. **Reducing number of markers to avoid confusion**
   If we use a single scene to show all the activities of all the topics then we'll need more than 15 markers to represent the objects in AR. Having multiple scenes gives us the opportunity to use a single marker in all the scenes representing new objects in new scenes. Which drastically reduced the number of markers to 6 in our case.

5. **Hide the physical markers**
   The tracking algorithms of the Vuforia - which is responsible for detecting and tracking markers and displaying objects on top of it, needs unique images with multiple trackable points to be tracked. Because of which QR codes become one of the most suitable markers. But semantically it doesn't hold any meaning to the user rather stageers them. This issue is solved using a superimposed image which replaces the actual marker once it is being tracked. This image can be used to hold relevant information about the orbital that it represents.

Fig 22. Covering the marker with informative image

6. **Using sound effects for auditory feedback**
   Sound effects on interactions can add another level of feedback after visual and haptic feedback, which will remove any remaining communication with what's happening in the scene.

7. **On screen textual instructions**
   Though the major instructions and study materials would be available in the booklet, but few microinstructions can be displayed over the screen so that users do not need to switch between the device and booklet to read instructions. This same thing could also be communicated through audio.

Final Ideas

In contrast to the double diamond design process, the ideation phase of this project follows a developmental process in which the ideas are constantly modified or changed based on the feasibility of the prototype development.

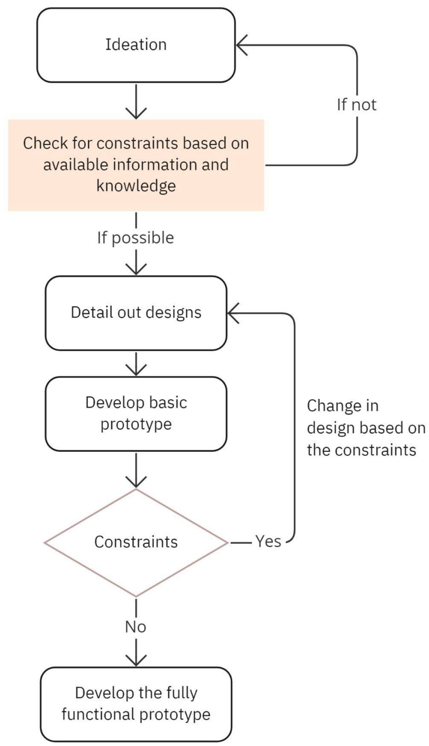


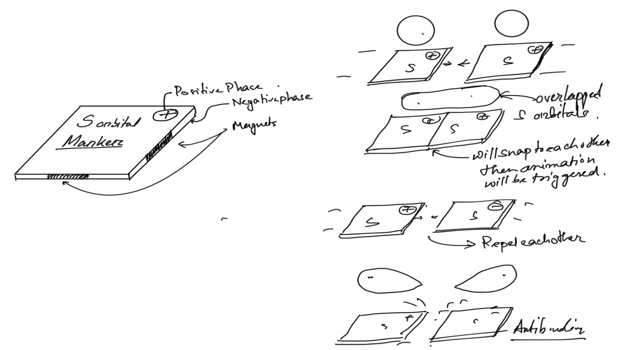
Fig 23. Ideation Process

Though the first set of ideas are brainstormed without considering much about the developmental constraints, But as the development phase begins, these ideas are constantly modified or improved based on the constraints faced while programming the solution.

The final set of ideas according to the topics are as follows

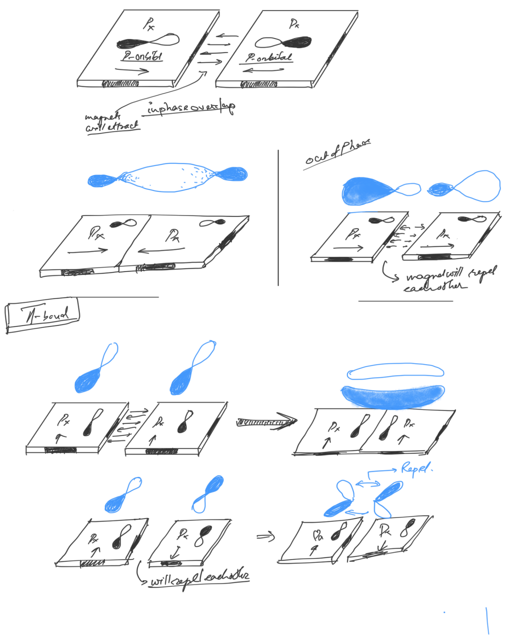
Overlapping of s orbital

1. Two 2D markers to show two s orbitals
2. On each of their backside another markers will be there representing opposite phase of the orbitals
3. When same phase markers come in contact then they will be snapped to each other and if the markers are of opposite phase then the user will feel the repulsion between the markers in their hands
4. Respectively new bonding or antibonding orbital formation will be displayed in the device screen



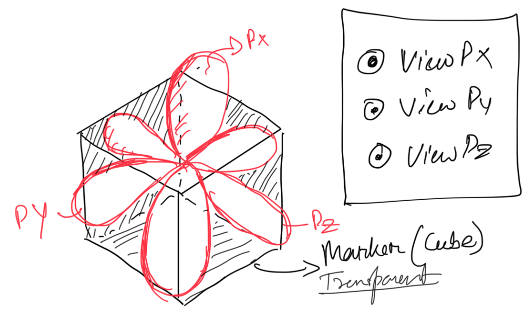
Overlapping of Px orbital

1. Two 2D markers to show two dumbbell shaped Px orbitals
2. When they come in contact with similar phases facing each other, magnets will snap to each other, showing the newly formed bonding molecular orbital
3. Rotating one marker 180 degrees will give antibonding molecular orbital
4. Rotating both markers 90 degree, that is side by side overlapping of the p orbital will give Pi bonds



Displaying the arrangement of all the P orbitals together in 3 dimensional space

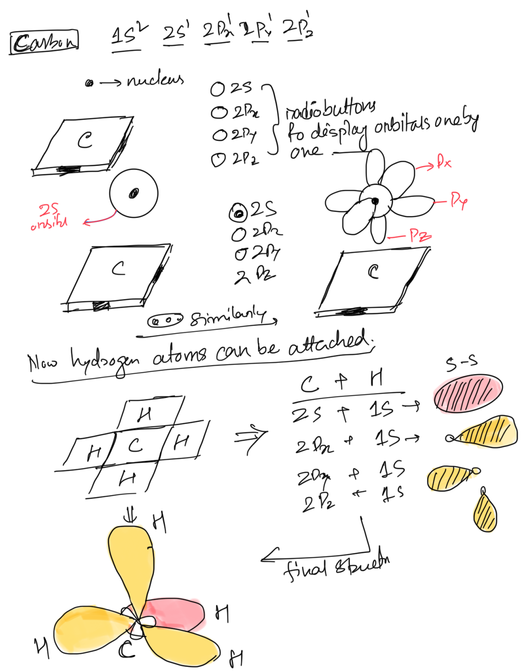
1. A cube marker to show all the three p orbitals, that is px, py and pz
2. With the help of Radio buttons each of them can be viewed in isolation
3. Rotating the cubes will show different orientations of Px, Py, Pz orbitals overlapping with each other.



Need of Hybridization through example of methane

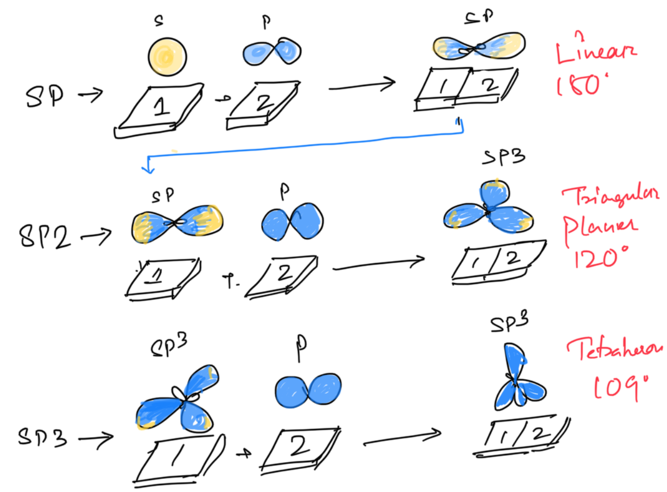
1. Carbon’s electronic config of excited state will be displayed on the device, based on which the student needs to form the carbon atom's orbital structure
2. Markers of hydrogen atoms when attached to each of the orbitals, they will overlap with each other

3. The final structure of the molecule can be compared with the original one to show the problem and how hybridization helps to explain it.
4. Explanation of why hybridization comes into place will be written over the booklet.



Process of Hybridization

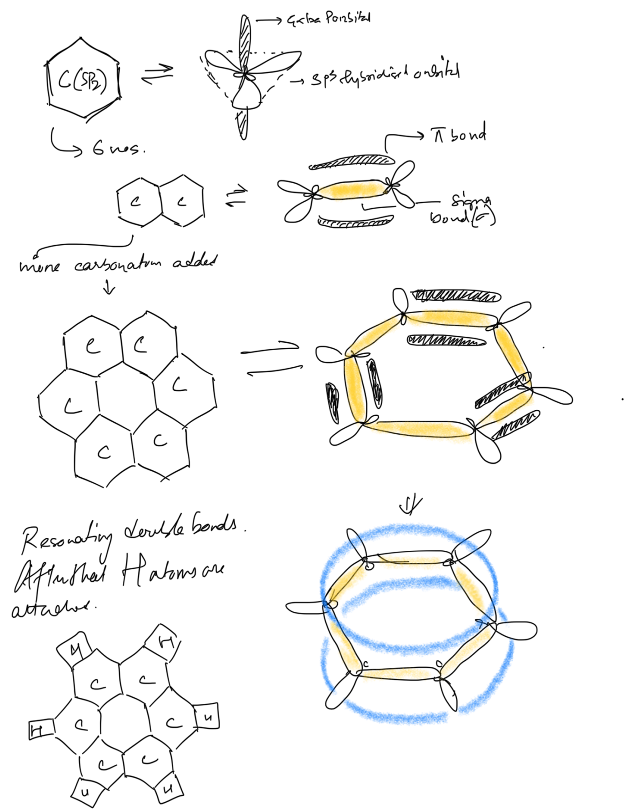
1. There are three types of hybridisation that s and p orbitals can form, which are sp, sp2 and sp3
2. With the help of two markers and three scenes all the three hybridization types could be shown
3. Details about the structures will be highlighted in the screen as well as booklet itself



Application(Benzene)

1. 6 sp3 hybridized carbon atom markers will be available, students have to make a ring out of it.
2. As they keep adding the atoms they'll see Pi bonds and sigma bonds forming.
3. One more concept resonance will be introduced when all the pi bonds move in a ring to give the resonance effect

4. At the end hydrogen atoms are to be added to complete the molecule
5. Toggle buttons could be given to visualize the structure in different forms like ball and stick.



Prototype Development

The prototype needs to be developed in Unity software along with creating the tangible markers and the booklet. The whole prototype developing phase can be divided into four main parts

1. Designing and making the Markers
2. Designing flow for the AR Application
3. Coding the interactions in Unity
4. ,Designing the Booklet

Markers

There are only two types of markers as mentioned earlier, the plane markers and the cube markers. A total of 6 markers are made that are sufficient across all the chapters. Again QR codes are used for giving unique identity as their detection and tracking are very accurate by the software.

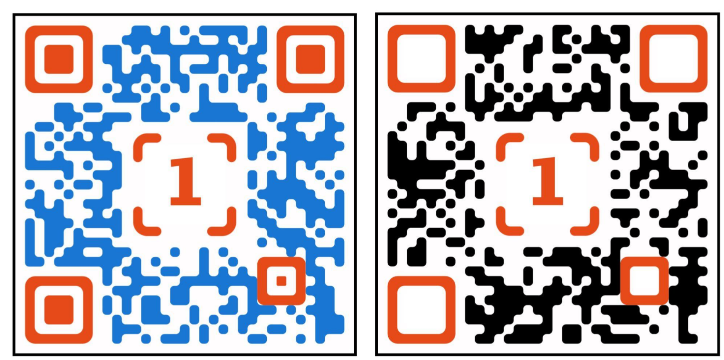


Fig 24. Plane Markers

To make these QR code based markers look visually appealing colors are added to them. Colors also help them to distinguish between two opposite phases of S orbital.

The markers are made of Foam Boards and each of their sizes are kept 6 cm by 6 cm considering the ergonomics of the students hand.. Each side of these markers have small magnets that are inserted.

Magnets

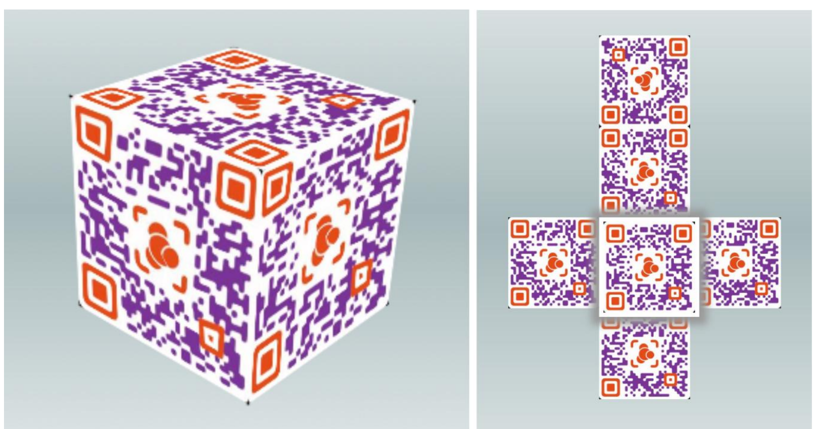


Fig 25. Cube Markers

Flow Design

The flow of the AR application is designed based on the order in which the chapters need to teach. A detailed instructions of how to operate the application would be displayed on the screen before the actual learning activities starts. The flow diagram is shown below.

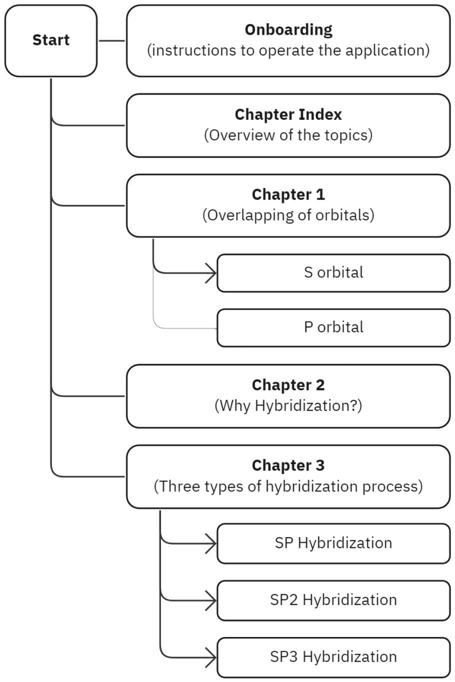


Fig 26. Flow Diagram of the AR Application

Coding the interactions

After creating the markers and flow and also the 3D models of the orbitals which are basically simple spheres and dumbbell shaped objects, we need to figure out programming the whole interaction of markers and assembling all the scenes together in a single AR application. Two tools have been used to build the prototype.

1. Unity : Unity is a game engine popularly used for game development. It is also used to develop games and applications using AR and VR.

2. Vuforia : Vuforia is a software development kit (SDK) for creating Augmented Reality apps. From creating the markers to detecting and tracking them in the application is taken care by Vuforia Engine .

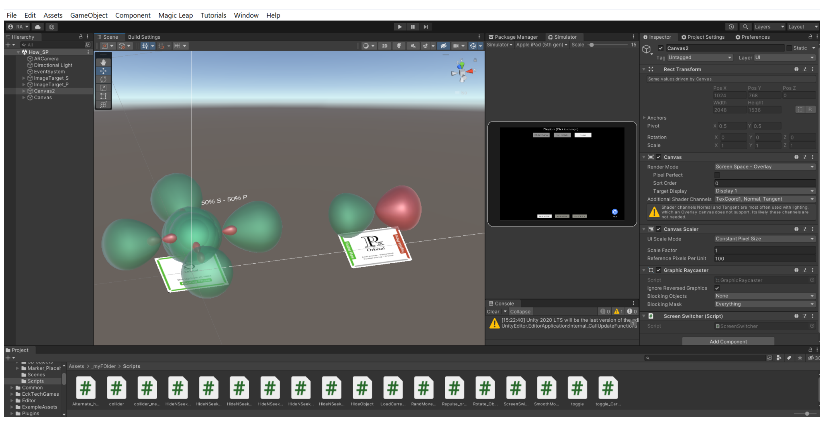


Fig 27. A view of the project setup in Unity

Links to the recorded videos of the prototype can be found in the below link.

Prototype links

Before going into the technical details let's get familiar with two main working elements of Unity.

- **GameObject:** GameObjects are the fundamental unit in Unity that represent almost everything inside the engine, may be characters, props and scenery or just a sphere or a box in our case. They do not accomplish much in themselves but they act as containers for Components, which implement the real functionalities. In our case each of the orbitals are a gameObject.

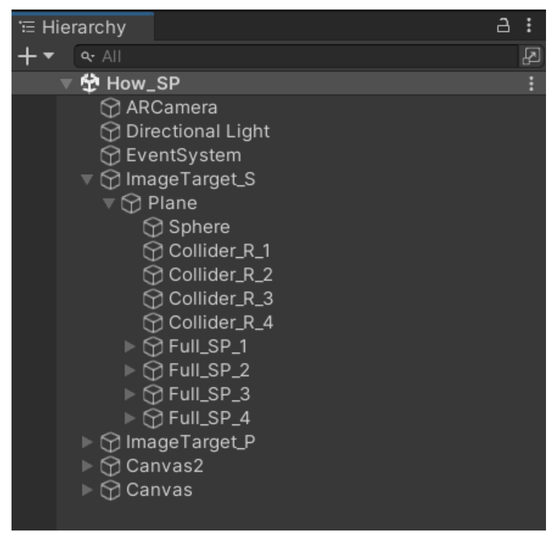


Fig 28. Game objects arranged in hierarchy

- **Collider:** Colliders are components built into Unity that provide collision detection using their various geometric 'Bounding Boxes' like sphere, box etc, the green lines shown surrounding the tree in the below image.

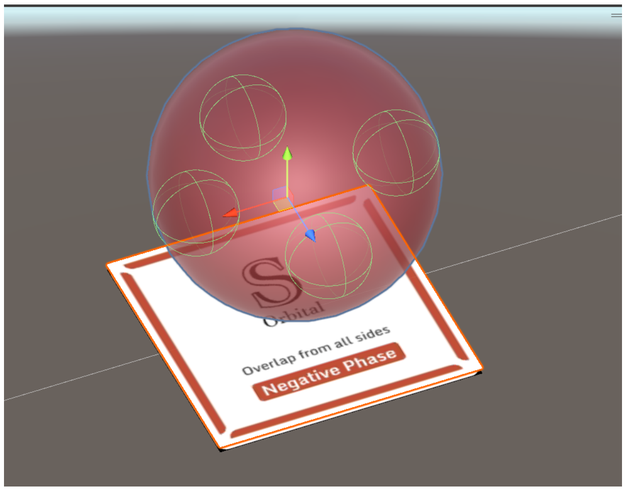


Fig 29. Sphere colliders(in green)

Colliders are the ones that trigger events when they touch any other colliders. And when these events trigger, with the help of code we can do anything like changing other objects, playing animations or anything that is part of the scene. I used these collider event triggers to build most of my interactions.

Now let's look at some of the interactions and how they have been developed in unity.

Attraction and repulsion

At the heart of all the interactions across the three chapters is attraction(In-phase overlapping) and repulsion(out of phase overlapping). The working principle behind how it is implemented in Unity using GameObject and colliders is quite simple. We have mainly four components inside unity.

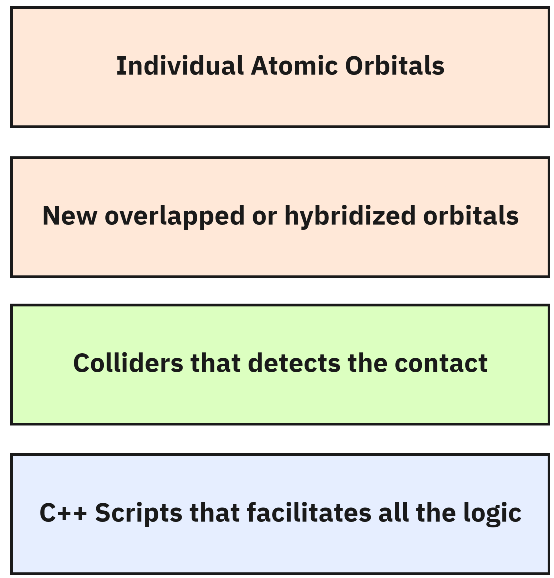


Fig 29. Sphere colliders(in green)

Individual atomic orbitals (s and p) and newly formed either overlapped or hybridized orbitals are all superimposed in a single marker as seen in the figure 30.

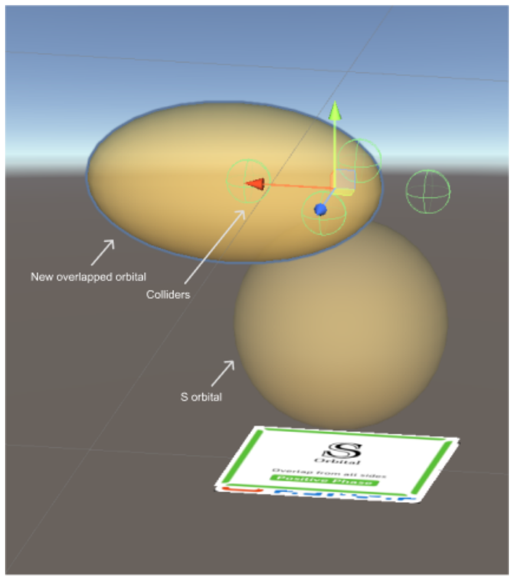


Fig 30. GameObject of orbitals and colliders

By default the new orbitals are set as hidden, they only appear when colliders collide with the right colliders of other orbitals, at the same time the individual atomic orbitals are hidden as soon as colliders trigger when markers come in contact. If markers again go away from each other the trigger goes away and the states of visibility reverts. This logic is illustrated through the diagram in figure 31.

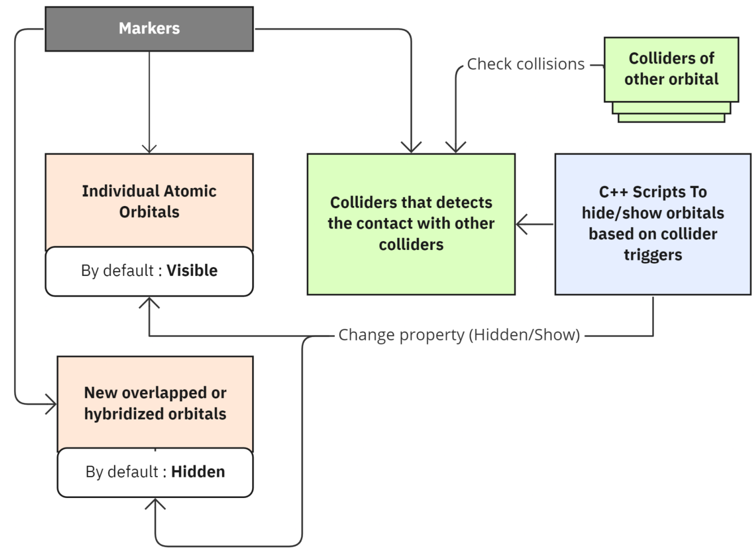


Fig 31. Flow visualization of the logic

Supported by this principle logic, we build and modify more interaction logics for different scenes. Handling s orbital is comparatively easy. Because of its non directional nature any collider can collide with all the other colliders of another s orbital. But for P orbitals which have directional nature, each of the colliders have to be tagged and coded specifically to trigger if some specific colliders collide with them. On top of that for both Sigma and Pi orbitals need to be superimposed in the marker, making the scripting more complex.

Prototype

Prototype links

Some screen captures of the final AR application

Evaluation

The primary goal of this project was to find a suitable method for teaching the concept of hybridization to students of 11th and 12th standard, so that students' difficulties could be resolved. Augmented reality has been found to be useful in situations where spatial visualization is required. So the solution will be evaluated in two directions.

1. **Learning of students :** The goal is to see if students are learning this topic currently and there should be a significant difference in terms of learning engagement with this method in comparison to other methods of learning. Key parameters to be considered while evaluating the learning perspective are -
    a. Ability to clear the preconceived misconceptions and make better understanding of the concepts
    b. Student shall relate to the concepts at microscopic level

2. **Usability of the solution** : Usability evaluation of the solution is to see if all the interactions are intuitive enough to help students learn the topic easily, may it be inter-marker tangible interactions or onscreen interactions. Below parameters will be the deciding factors of this evaluation.
    a. Effectiveness of the haptic interactions
    b. Intuitivity of the onscreen interactions
    c. Effectiveness of Marker types (Cube markers vs. plane markers)
    d. Overall ease of use of the application

Experiment

I tested the final product using an experiment that addressed both usability and learning issues. **Three students who are all in class 12** and who learned the subject six months ago are recruited for the study. The experiment can be divided into these steps,

1. Get familiar with the students and tell them about the project and the motive of this study
2. Pre-test questionnaire(pen & paper) based on the current knowledge
3. Printed booklets were given to read the text and do the activities on their own by following the instructions
4. Observations on usability were noted down(difficulties, moments when help needed, surprise and satisfactory moments etc)
5. Post-test questionnaire (Few Q. were same as Pre-test)
6. Feedback and discussions on usability, new learnings and design inputs

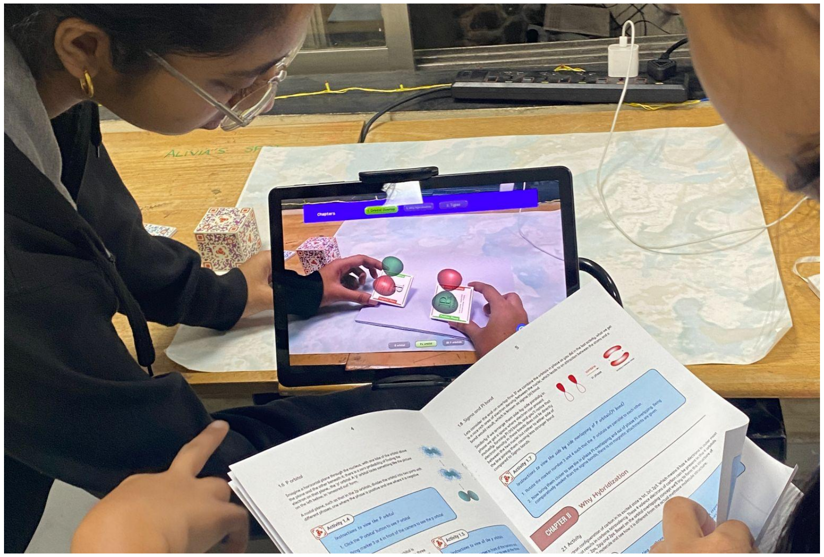


Fig 32, 33. Students trying out the final design

The learning aspects are evaluated based on two tests that were conducted before and after using the product. These tests were a series of questions that tested the candidates' conceptual knowledge of the concepts related to orbital hybridization.

Pretest questionnaires -

A. Do you love chemistry? Rate your interest in chemistry on a scale of 5.
B. What are the topics in your current chemistry course that you love and the topics that you find difficult.
C. Write your understanding of atomic orbital. What do you mean by Phase and Node of orbital?
D. “Electrons move inside an orbital in a defined path” - Is this statement correct?
E. What do you think the bonds between two atoms look like?
F. Can you define Hybridization?
G. What is the need of hybridization?
H. What are the types of hybridization that S and P orbital can form?
I. Did you understand the topic when it was taught in your school/tuition? Or you need help from other sources like books, external videos etc?

Post test questionnaires -

A. What is your understanding of atomic orbitals now? What do you mean by Phase and Node of orbital? How many phases and nodes 1s and 2P orbitals have?

B. What do you think the bonds between two atoms look like?
C. Define Hybridization.
D. What is the need of hybridization?
E. Can S orbital form Pi bond? Give a reason.
F. Why do the shape of the orbitals after hybridization change?

I also showed my design to some school students and asked them to try it out and provide honest feedback. I went to a nearby school and demonstrated the whole thing to a group of 12 students, four of whom came forward to try out the design. During the time, I took notes on the key observations and also asked a few usability questions.

Fig 34. Students trying out the final design

Result

Students Learning : All the students were well-versed already which we can tell from the answers they wrote for the pretest questionnaire, still improvements were seen on a few topics like node and phase of orbitals, bond formation, orientation of P orbitals, need of hybridization. They found the booklet very simplified for understanding. One of them mentioned "Best way to visualize chemistry topics", while another student said, "Will be beneficial just after learning in school, not recommended as a primary tool to start". Which was already my motive to use it as a supplementary learning material to clear the misconceptions. One of the key suggestions was to include the d and f orbitals which are more interesting and complex to visualize.

Usability : I received overall positive feedback on the usability of the design from both experiments. The interactions are quite intuitive with the help of instructions, and students were able to complete the tasks with ease. The following are some of the evaluation's positive findings:

1. Students found magnetic snapping and repulsion interesting(tried out multiple times).
2. Cube markers are preferred over plane markers. The main reason for this is that cube markers are always trackable, whereas plane markers are not detected once they are out of sight.
3. Found the 3D models realistic.
4. Able to handle the markers properly on their own. First

few times they faced problems but they learnt it on their own from the mistakes,
5. The UI is easily navigable. Once all the activities finished students tried out previous activities by clicking on the respective buttons and checkboxes.
6. Did few activities for 2nd time without looking at the instructions, like formation of methane structure
7. Brought the markers closer to the camera in order to look at the written content

On the other hand, there were some negative insights that needed to be worked on and resolved.

1. Opposite phase markers were difficult to handle with one hand. This occurred due to marker repulsion; using only one hand did not provide much contact between the markers, causing the 3d models of orbitals to not change their shape.
2. Students found a few Instructions confusing
3. Difficult to do in sitting position and in group

Discussions

The purpose of this project was to see if augmented reality could aid in the comprehension of complex scientific concepts, particularly in chemistry, where a high level of spatial visualization is required. We also looked at the intuitiveness of interacting with this new technology through various markers. As seen in the evaluation results, the outcomes support our goal in terms of the ease of use of the technology by students, indicating that it can be used as a new medium in schools to teach difficult concepts. Students have found design interventions such as magnetism, overlaying markers, and the use of 3D markers to be useful. Students enjoyed 3D markers and magnets with haptic feedback. The information about orbitals written on the markers was also very helpful. All of these positive responses validate our design as a viable method for school education.

There were some limitations in evaluating the learning side of the design due to the absence of our primary user group in evaluation, which are students who struggle with spatial visualization. All of the students I evaluated my design with are already well-versed in the subject. A more sophisticated screening of users was required prior to conducting the evaluation. This will provide more valuable learning insights.

Finally, this project helped me realize the potential of augmented reality as a tool of learning and how the different features of the design could be extended to various fields of education.

Learnings and Reflections

1. Solving a problem from scratch, getting the final output in hand and finally testing it with real users was real satisfaction. I thoroughly enjoyed the whole process and learnt lot's of new things during this project.

2. After spending a good amount of time researching what's happening in the field of augmented reality and developing a complete application through programming the interactions, I realized the creative potential of AR.

3. During this project I learnt unity from scratch and explored the core interactions, which will help me in future to develop coded prototypes in the field of AR/VR and Game development.

4. I gave much time to research about the problems of students when the problem was already known. In comparison to the time given for research the insights were not that much.

5. There should be multiple iterative rounds of evaluations in order to know the shortcomings of the solution and rework on it.

Future Scope

1. An extensive rapid user testing and prototyping need to be conducted to find out issues and bugs in every use case of every scene.

2. Creating a DIY kit for the markers so that anyone can make the markers using the template and make use of the application from anywhere around.

3. Examples of benzene could be developed in the project due to shortage of time, so need to incorporate that in the solution along with a few more examples.

4. Will try to use animations when gameobjects change from one shape to another, which will be more intuitive to learn.

5. Supporting learning materials that are now written in the booklet, can be combined with the application itself.

References

1. Nakiboğlu, Canan. “Instructional Misconceptions Of Turkish Prospective Chemistry Teachers About Atomic Orbitals And Hybridization.” *Chemistry Education Research and Practice* 4 (2003): 171-188.
2. Wu H. and Shah P., (2004), Exploring visuospatial thinking in chemistry learning, *Sci. Educ.*
3. Al-Balushi, Sulaiman M., and Sheikha H. Al-Hajri. “Associating Animations with Concrete Models to Enhance Students' Comprehension of Different Visual Representations in Organic Chemistry.” Chem. Educ. Res. Pract. 15.1 (2014): 47–58. Web.
4. Abdinejad, M., Talaie, B., Qorbani, H.S. et al(2021). Student Perceptions Using Augmented Reality and 3D Visualization Technologies in Chemistry Education. J Sci Educ Technol.
5. L Ya Midak et al 2022 J. Phys.: Conf. Ser. 2288 012017
6. Sarah E. Wegwerth, Jason S. Overby, Christopher J. Douglas, Julia E. Winter, Gianna J. Manchester, and Joseph EngalanJournal of Chemical Education 2021 98 (2)
7. F. Cortes Rodriguez, L. Krapp, M. Dal Peraro, L. Abriata, Chimia 2022, 76, 145, DOI: 10.2533/chimia.2022.145.
8. Mobile Marker-based Augmented Reality as an Intuitive Instruction Manual, HANNAH REUTERDAHL
9. NCERT SChemistry Textbooks of class 11 and 12
10. ORGANIC CHEMISTRY by Jonathan Clayden

- END -