

Hello, welcome to the course on the Physics of Functional Materials and Devices. I am Professor Amreesh Chandra from the Department of Physics at IIT Kharagpur. I am the coordinator of this course on the Physics of Functional Materials and devices. This is the first lecture of this course. So, let's start with the basic introduction, and then we will give you a brief overview of the various topics that will be covered in this course. In today's lecture, these are the basic concepts that will be covered.

Introduction, classification of materials, what are functional solid-state materials, the different types of functional materials and finally, we will give you the various applications of these functional materials. In the details of the course, I must answer this question that is, why the choice of the topic which is given, that is the physics of functional materials and devices. And how are these things related? Because they can also be independent terms and they can form an independent course. So, you are trying to bring three terms together and make a course out of it.

How do we relate these terms and then what are the things which we are going to follow in this course? So, we know physics is what? It is a subject that deals with the science of matter, motion, and energy. Energy is both the utilization and transport of energy. What is a material? Material is something which is made up of matter, made up of matter and the subject which deals with the science of matter is what? Physics. So, we have at least two common terms there and hence physics of materials seems to be a very logical topic. But why are we putting the term functional into it? Why are we not saying just the physics of materials? And the answer to this lies in a very common question.

which all of us that is people working with materials, chemistry, physics of materials, material science, and metallurgy, we all have to answer. What is that question? People ask what the application of your material which has been synthesized by your team in your lab or the industry. What is the use of this? This is a common question which is asked to all of us who are working in materials. So, we have to answer that question. We find and we give one application. The next question which is a follow-up question you are making a material and you are only using it for one application.

Then what is great you are doing? You can make a material that can be used in more than one application and that is where the use would be. And that is where the term functional comes into the picture. Functional materials are a class of materials that have various types of functions or applications but with at least two or more than two types of functionalities. That means you have a material that can have functions like it can be used as a dielectric, it can be used as a dispersoid, it can be used as a sensor, but a functional material should have the capacity that it can be used in two applications without the requirement that you need to change the state or the phase of the material. For example, if you look into multiferroic ceramics which are common terms that are being used and you will hear a lot when you go forward in the field of material science or physics of materials, these are the materials that can be used to detect electric or magnetic field variations.

That means they can be used as electric field or magnetic field sensors along with that they can be used as a dielectric in a capacitor in a conventional capacitor. so, the same material, for example, bismuth ferrite. It is a common multiferroic ceramic, it can be used in electric field sensors, it can be used in magnetic field sensors and it can be used as a dielectric in capacitors. So, one material with three applications is what we want and that is why we add the term functional before materials looking at the requirements of today's world. So, conventionally people talk about the topic of the physics of materials, but if you look into the requirements of today's world we add a functional term and therefore, this course is called Physics of Functional Materials and Devices.

What is the most common functional device which you see around, it is your mobile phone. If you look into the capabilities of that mobile phone. It can be used for communication. Most young people use mobile phones for the camera, they use it for audio player and audio recorder. It can be used as a torch or a projector then a document scanner and many many more applications which just growing with each passing day.

You have a new mobile phone, new functional, but when you go from talking on a mobile phone and then using it as a camera do you need to change anything in the mobile

phone? No, you do not need do not need to change the state or the phase or the design of the mobile phone, everything is integrated and therefore, it is a smart and functional device. So, we will be talking about a lot of materials in this course that would be used for at least two applications or more than two applications and that is why this course is called as physics of functional materials. If you look into the type of materials that we have been studying since school days, there are three types of classifications or categories in which we talk about the solid state, the gaseous phase, or the liquid phase of a system. You have solid materials, you can have liquids or you have gases and each of them is classified by certain properties. For example, solids are classified by definite shape, definite volume, and definite mass and they are associated with high densities.

As we move from one category to the other, you will see that certain properties will go on getting eliminated as we move from one to the other. So, if I go to liquid, liquids are not associated with definite shape, they take the shape of the container or the enclosure in which they are confined. So, the definite shape term goes out of the picture. Similarly, for gas, the two terms that go out of the picture are definite shape and definite volume, but they are associated with definite mass and they are considered to have low densities. If I go further and talk about solids that have well-defined shapes or volume associated with those shapes, these are characterized by features such as they are incompressible, they are rigid and they are considered to have high mechanical strength.

What is happening in solids? In solids, we consider that the atoms or the molecules are closely packed. So, they are closely packed and these two atoms or molecules are held together by strong forces so that they cannot move randomly. So, there are no random motions that you see in solids. These solids may not allow any random motion of atoms or molecules, but it does not mean that these atoms and molecules are static. They have certain motion around the mean position where they are sitting in the lattice of the solid.

So, there is some motion around the mean position. Based on the atomic arrangements, the solids can also be classified as single crystalline, polycrystalline, or amorphous solids. What are these? Single crystal means it is only one small crystal. No, it does not mean

that there is only one small unit cell in the lattice. It means that the growth when you start putting atoms in the at the lattice points and then you start building up the whole structure, the growth of the material is such that it is in one of the preferred directions.

And the growth is such that everything is well-ordered. So, you will put the atoms layer by layer, layer by layer and if you see that you are making a crystal which is a single crystal, but along the C axis, then all the atoms would be arranged in the C direction and the growth will occur in the C direction. So, if you look into the periodicity of atoms, this will extend throughout the material. So, you will have a long-range ordering with periodicity extending throughout the material. But these are not very common examples.

You do not see single crystalline materials routinely. What you see is the polycrystalline materials. What are polycrystalline materials? These are materials, that have long-range orderings, but it does not mean that it is throughout the materials. They have to order in such that you have small crystallites which means, you have small regions that have well-defined boundaries, and around inside this region you see the ordering which is similar to single crystal ordering. But when you move from one small region to the other, the two regions may be differently oriented.

So, you may have this region, you may have the other region. In a single crystal, both of them are aligned in the same direction and the growth is occurring in the same direction. But when you go to polycrystalline, this region may be randomly oriented to the other region, And these small crystallites are known as grains. But the unit cell is the crystalline nature of the lattice that is forming inside these grains are similar. So, you may have the same tetragonal lattice or arrangement inside this grain and the same tetragonal lattice or arrangement of atoms within this grain, but these two grains may be arranged in a manner that they are not aligned.

They can be random or they can have certain orientation which is different from each other. So, these are polycrystalline materials and this is what you routinely see in nature and all around. Then the third class of materials that is amorphous materials, here the

arrangement of atoms is such that you have short-range ordering. So, you can go on putting atoms, but the ordering of these atoms would be in a small region and if you move from one region to the other, the ordering will be different. How do we differentiate between long-range ordering and short-range ordering? Which parameter tells me that this is long-range ordering or short-range ordering? This will be discussed in the following classes when we start talking about the crystalline nature of the crystals which are formed using different kinds of atoms.

You can also divide the materials based on the energy band gap. You have heard that, in semiconductors, the valence band and the conduction band are separated by a gap which is called a band gap or to be precise energy band gap. Based on the nature of the energy band gap, the materials can be classified as metals, semiconductors, or insulators. And please note what did we just say? We said based on the energy band gap. So, what is the magnitude of this gap that allows us to differentiate between the three classes of materials? If you look into metals, the band gap that is associated with this kind of material is 0 or they have no band gap.

The conduction band and the valence band are just overlapping. So, there is no band gap. If you look into the insulators, these are materials that have a band gap of magnitude which is more than 3 eV. Whereas semiconductors are the class of materials that are intermediate to metals and insulators, they have a band gap let us say from 0.1 eV to 3 eV or slightly less than 3 eV.

So, based on the band gap you can classify materials into three classes, those are metals, semiconductors, and insulators. Various types of conventional materials are being used in today's world. devices which are You have various using these kind of materials. These can be transition metal oxides, you can have transition metal sulfides, you can have metal-organic frameworks which are called MOFs, you can have conducting polymers or you can have various forms of carbons, you can have different forms of different forms of carbons. So, why does the property of a given class of material differ from the next? Let us just take the arrangement of atoms in two of these subclasses.

Let us say the MOF that is a metal organic framework and transition metal sulfides. Without going into details, let me just give you a brief overview of the reasons why the properties of these two materials would be different. The details will come in the following lectures because first we should know how to synthesize these materials and then we will discuss the change in properties and the reasons that drive this change in properties in such kinds of materials. So, you can see that the arrangements of atoms in MOFs are very different from those in transition metal sulfides. Therefore, suppose I have to have a scattering of an atom or a ray from such kind of transition metal sulfides and the same kind of beam, be it an electron beam, or be it an x-ray beam, is incident on the metal-organic framework.

The response of these two materials would be very different from each other and hence the diffraction or the scattering which you will see would be different. Hence you can make two different kinds of detectors which can be wavelength detectors using these two materials. This is a very rough explanation of the reasons why the properties of these materials would be different. We will discuss each of these points in detail as we go along in the course. So, till now what you saw was that we discussed the materials which are conventional solid state materials.

Let us go a step further. What is that step further? That is what are functional solid-state materials. Conventionally the term functionalization is used. What does the term functionalization mean? The term functionalization means it is a process of adding new features, functions capabilities, or properties to a material by changing the surface chemistry of the materials and without changing the overall phase of the materials. But nowadays sometimes people also use the term that functionalization can be associated with a slight change in the phase of the material. Which phase am I talking about? Please remember the definition of the term phase is a phase of a material is what? It is a state that is physically distinct, chemically homogeneous, and mechanically separable.

So, you have a chemical formula of a material, for example, ABO_3 which is a perovskite material which is a well-defined material having an arrangement of atoms. So, if you look

into the arrangement of the atoms in ABO_3 you can see that the A atoms are at the cube edges, the B atom is at the body center whereas, the oxygens are at the phase centers. So, these have a well-defined physical characteristic, and if you choose another material which is of this nature the atoms are arranged in certain order in a circular confined structure. These two are not equal and they can be separated using certain mechanical processes. It can be a centrifuge you have certain precipitated particles surrounded by water droplets.

So, you can separate these two phases using a centrifuge it is as simple as that. So, this is the term functionalization. So, once again what is functionalization? You must understand and remember this definition clearly. Functionalization is the process of adding new features, functions, capabilities, or properties to a material by changing the surface chemistry of the material. Functionalization can be of various types.

What can that be? It can be in terms of size or dimensions. So, you can have a very large material let us say it is 1 meter x 1 meter and then you cut it, cut it into small pieces and take it to 1 centimeter x 1 centimeter. What do you expect? These 1 meter x 1 meter surface and 1 centimeter x 1 centimeter surface both have the same kind of properties, will they have the same mechanical strength, will they have the same electrical properties, and will they have the same thermal properties? It is very clear that just by changing the size or the dimensions you can change the property of a material or you can change the properties of this material. That is what is called moving from bulk to nanomaterials or you can talk in terms of dimensions which means you are going from three-dimensional materials to two-dimensional materials to one-dimensional materials and zero-dimensional materials. We will just discuss these things in the next few minutes.

You can change the shape or the morphology. So, what is morphology? Morphology means the shape of a given particle in a material that is the morphology of the particle, but shape can be the overall shape of the material that you are talking about. So, you can have solid spheres or you can have hollow spheres, you can have a rod, you can have solid cylinders, you can have hollow cylinders, you can have cactus, you can have any

kind of structures which can be formed and when you go for example if I have a material like this which has a triangular shape and then I have a material which has a spherical shape, will they have the same response? Logic tells us these are two different well-defined shapes which means the particles have different shapes and their response characteristics should be different. So, they will not have the same properties. So, by changing the shape or the morphology of the particle you can change the properties of these materials. You can change the porous structure of these materials.

For example, you can have materials that are very closely packed or you can have materials that are loosely packed. What do you expect? Will this material have the same response as this material? No, you can see that the gap between the two atoms that are there in this kind of material is very different to that in the earlier case and therefore, the properties of this material would be very different. Properties like what? Diffusion. What is diffusion? Moving of mass from one region to the other region. So, if you have regions that are vacant spaces then the mass can travel.

So, the diffusion processes are expected to be very different in porous networks with different orders of porosity in them. Similarly, by changing the doping of a material you can change the conductivity of a material. It can be thermal conductivity, it can be electrical conductivity. So, you can have different kinds of materials and you will get a change in the conductivity.

As I just said moving from bulk to nanomaterials. What is a nanomaterial? Everybody uses the term nanomaterial. How do we define it? The definition of a nanomaterial is that it is a class of materials that has at least one of the dimensions in the range of 1 to 100 nanometers. What do we mean? So, if you have the 3 axes and you make a material. So, what is there? You have the x-axis, the y-axis, and the z-axis.

So, 3 dimensions of a material. If the dimension of this material is in the range of 1 to 100 nanometers in at least one of these dimensions. So, let us say the dimension on the x-axis is 300 nanometers, whereas on the y-axis it extends up to 500 nanometers, but on the

z-axis, it extends only up to 10 nanometers, then it is a nanomaterial. The same thing, if in the x direction, the dimension is 1 meter, in the y axis the dimension is 2 meters, but in the z axis it is only 50 nanometers, then also the material will fall in the class of nanomaterials. Nano means a billionth.

So, that is 1×10^{-9} meter, ok. That is what nanomaterials basically means. And Richard Feynman is considered as the father of modern day nanotechnology and in this course we will be talking about a large number of nanomaterials. And the foundation stone for the modern day subject of nanotechnology was actually placed by Feynman during his famous lecture in 1960 during a APS meeting, where he said there is plenty of room at the bottom. That means, as you go on reducing the size of the material, novel physics can evolve if these small sized or nano sized materials are carefully investigated. This can lead to change in melting point, the surface energy or surface area, the electrical properties, the mechanical properties, the optical properties and magnetic properties.

You can have changes in these properties. This is what he indicated and we are exploiting this concept extensively in today's research and the devices which we are making and we will be discussing them in this course. You can have various types of nanomaterials, means a three dimensional material is what? What is a three dimensional material? It is a bulk material. That means, all the three dimensions are more than 100 nanometers. If you go to two dimensional materials, then what is happening? You have at least two dimensions which have the order which is more than 100 nanometers, whereas the third axis is confined that is the dimension in the third axis is 1 to 100 nanometers. Then you have 1D materials, what are those? 1D materials are the which have one of the axis which extends to more than 100 nanometers, whereas the other two dimensions are such that they have range in the order of 1 to 100 nanometers.

And if you have a material which have all the three dimensions in the range of 100 to 1 nanometer, if you have a material which has the dimensions in the range of 1 to 100 nanometers and this is true in all the three dimensions that is in the x axis, in the y axis or in the z axis, the dimension is in the range of 1 to 100 nanometers, then it is called as 0D

materials such and most commonly you use those terms as quantum dots or 1D materials could look at nano rod type structures, nano wires, nano belts, nano tube kind of structures. Similarly, for two dimensional materials, you can have nano plates, nano sheets, nano walls or nano disks. So, you can see the various types of materials which are there. So, you can see all the various types of materials which are there. So, if this is just a cartoon of the different kind of arrangements which lead to various kind of materials, you can clearly see the properties of various types of materials are expected to be different because the shapes are very different and therefore, the properties of the materials which will have these kind of particles would be very different.

You can have the change in the dimensionality which was exploited extensively in carbon, carbon which is well known for many centuries now, but still lot of work is being carried out in this structure and you have got people who have got Nobel Prize just by tuning the structure of carbon and getting new forms of carbon. So, for example, graphene was discovered in 2004, carbon nanotubes in 1991 by Yajima and fullerenes in 1985 and you have various kinds of arrangement and you have these materials being used for different applications. Graphene discovered in 2004 and the discoverers were given Nobel Prize in 2010 itself. These kind of materials can be used for ion detection, molecular recognition, disease diagnosis, they can be used for energy storage devices, device modeling, thin film electronics, actuators, electromagnetic shields and they can also be used in medicine, food industry and many other applications.

This is where I give you the first assignment of this course. I have been talking about how the discoverers of various forms of carbon have received Nobel Prizes. I could have mentioned this on the slide itself, but let me give you an assignment very simple one. Please find out the people who have received the Nobel Prize by working in the field of carbon structures and why these people were given the Nobel Prize. What was the special structure that they made using carbons that led to the award of the Nobel Prize? So, you should try to find out and you will see that it is not that you have to make complicated structures to get very high-performance materials, you can get very simple structures and they will have enormous applications.

The next could be in the shape of the particles. You can see that these are various types of particles. Do they look the same? No, not. Some of them are hollow, some have a cactus-like structure, and some have a rose-like structure. So, these are real particles of material. So, these are cobalt oxide, this is chromium oxide, this is sodium iron phosphates, this is sodium titanate, this is capped carbon.

And if you look into it, if I put all these particles in front of you, you will say that they are all the same. But if you take a high-resolution picture, which is obtained using a scanning electron microscope, the shapes are very different of these particles. The shapes are so different that their properties would also be different. This is what is meant by functionalization in morphology, which induces the change in properties and that will be discussed in the course as we go along. So, you can have different cavities, you can have higher active sites because the surface area is very high or you can have well-defined channels for the ion or any kind of charge carriers to move along the surface of a particle, which can be used in a device and that is what is being used in today's world.

You can have composites. What does it mean? You make two different materials to come along, and make a composite and the property of this composite would be different from that of the individual component. That means, for example, you take MOF, MOF is like these brick-shaped particles and then you take a conducting polymer like polypyrrole. You can see this is the shape of a polypyrrole and then you mix it, you make a mixture. They both exist in their shape, individually they will have their properties, but when you mix them the overall structure will have very different properties from that of the individual components and that is what is done in composites you can make new properties by having the mixtures of these two systems. I have talked to you about various classes of materials, but how do you make these materials? It is essential that if you want to do good physics, get your chemistry right.

That means, making materials that are single phase, which have the desired molecular formula and you do not have impurities in these materials. That means you do not have a secondary phase in these materials, you do not have a system that is not stoichiometric. That means, if I have to get ABO_3 structure, then it should be ABO_3 . It should not be AB_5O_3 minus delta kind of a structure that is chemically unstable.

So, you must get your chemistry right if you want to do good physics. Therefore, you must know the various techniques that are there to synthesize these materials. So, we will be talking about two classes of synthesis protocols. So, all the synthesis protocols are sub-classified under these two headings, either bottom-up or top-down. So, we will be talking about a large number of synthesis protocols to obtain the materials that are going to be used in devices. These devices would use the materials which are synthesized using various techniques.

These devices would be useful for at least two or more than two applications. The various applications that we will be talking about can be electromagnetic shielding and electromagnetic sensors, you can talk about lasers, you can talk about use in fiber optics or waveguides, and you can talk about their applications in car exhaust, and molecular synthesis. That means the catalytic properties of those materials. You can talk about the use of these materials in batteries, hydrogen storage, and supercapacitors, you can talk about super materials. You can talk about super materials means superconductors, supercapacitors, and giant magneto resistors materials.

So, these are materials that generally have the term super in front of them because they have a property that is known which means conductors are known, but superconductors are the ones that have much higher conductivity than conductors. That is why you add the term superconductors. Same thing with supercapacitors, capacitors, and supercapacitors. Capacitors have a capacitance in the range of milli to microfarads, but if you have supercapacitors they have capacitance in the range of farads to hundreds of farads.

That means, 10^6 orders higher. Therefore, the term super capacitor, or finally, you can talk about the magical materials which can have negative transport properties, you can have a negative refractive index or you can have metamaterials. So, these will also be discussed in this course. So, let me summarize the introduction lecture which was given today. We have given you an overview of the solid-state material, and how we associate the shape and volume with it depending upon the change in shape and volume or morphology or confinement, you can have different types of properties in these materials, and you can arrange atoms in a different order and you can have different types of materials, you can have single crystalline materials, polycrystalline materials or

amorphous solids. We have also given you the classification of materials in terms of the band gap.

This classification leads to a group of materials which can be classified as metals, then there is another group of materials which can be classified under the heading of insulators and finally, you can also have a group of materials which can be classified under the heading semiconductors. In comparison to the conventional materials, the functional materials that will be discussed in this course will have properties that will be higher than those seen in conventional materials, you will have higher physical properties, higher thermal properties, electrochemical properties, electrical properties, or magnetic properties which would be higher than the conventional materials. Finally, I have also discussed the importance of synthesizing these materials and why we should understand the various synthesis protocols that are there to obtain these materials. That is also important and we will be discussing it in this course.

These are the various books that are followed to make today's lecture. I hope you enjoyed the lecture and I thank you for attending this course on Physics of Functional Materials and Devices. See you soon. Thank you.