webinar 01 – setting the stage

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This is the first regular feedback webinar of this course. You have worked now for one week on the topics of week 1, which were meant to set the stage. And here today we will look back at this week and comment a bit on things you have reported. One of the things I asked you last week is who are you, and we can look at some results. There were about 25 people who wrote the self-presentation in the forum and who submitted an are you on board forum. A similar number subscribed to the Zulip channels, so this gives an order of magnitude to the number of people who are following the course. We are following this course in the synchronized version as it is happening at Flemish universities. These people are located at various places in the world. These are the people who registered for the course in the past 30 days, so the run-up to the start of the new academic year. As you can see, it spreads over different parts of the world. But this is not the end. When I was looking at this map this morning, I wondered, huh, I should maybe plot everybody who has ever started following this course, and that's statistics of now 8 years. And then it looks like this. So this really covers most parts of the world. Well, we are not with that many people simultaneously, but it shows that there is an audience, and people are using it. Far beyond the classroom where this course originally has been developed for. Some background about the people who are currently in the synchronized version. So age distribution, about one-half is under 25. Then more than one-third is between 25 and 30. And a bit sixth or so is between 35 and 44. Sometimes there are older people present as well, apparently not this time. And your background. There is, well, one-fifth, one-sixth is a bachelor student. Then more than one-quarter, roughly one-third is a master student. About one-quarter is a PhD student. And the remaining quarter is divided between postdoctoral researchers, staff scientists, people from industry, and a very interesting category, hobby learners. That I always like if people want to tackle a topic just because they find it interesting. I asked you, what are your hobbies? I asked you, what are your expectations? And that was fairly evenly distributed. So here you have the four questions I presented to you. To learn about the concepts of materials physics. To learn about the concepts of ab initio methods. To acquire hands-on expertise on using ab initio methods. And to be able to read papers that make use of ab initio methods. Well, these were, all of them, you found equally important. The magenta bars, they indicate that you rated this as very important. And, well, every topic seems to be as important. You could also write about your motivations in the forum. And I have collected some answers. So I read people who want to get to know some extra tools to use for computational, in computational physics, to improve my knowledge and skills. Also somebody who wrote, I'm an experimentalist, but I want to master these computational tools as well. So these are definitely obvious reasons why this course can interest you. There are also people with a chemistry degree. Who are already familiar with simulations, but only with isolated molecules. And who want to develop this skill towards crystalline materials. That we will be mostly studying here. So that too is a valid motivation. And every year there are a few people who take the course also with an interest on the teaching environment. How is this done? And can you maybe use parts of it? Can you maybe use parts of this approach for your own teaching? So that's always interesting too. And especially to those people, but to everybody. I invite you to comment on what it means for you as a student. Is there something that is particularly helping you? Is there something that I could do better or differently that currently blocks you? So that kind of input is always useful. Remember, I have a suggestion button for this at the front page of the course, as I explained in the introductory session. So that was a quick view at the background of the audience for this year. There were some questions on

the practical organization. I put here two very similar questions. Somebody who asked, well, there is in the text that campus students are expected to submit a weekly report. And what is meant with these weekly reports? And I must say this was an old wording. It escaped me that it was written like this in the frequently asked questions section. So I changed the wording now. But with weekly reports. I mean the collection of everything that you are asked when working through the material of that week. That can be answering on the forum or submitting a PDF or taking a multiple choice quiz or doing the hands-on parts of a given week. All of that is collectively, these are the tasks for that week. And how is that checked? Well, I verify manually for everybody, at least for everybody who is a four-credit student, whether or not these requirements are met. And the second question that you see here on the screen is very similar, just with a different wording. So are the assignments the Let's Play folder? Yes, that's part of it. These are the hands-on exercises. But it's more than that. It's also everything that is asked you to do when working through the material of that week. Somebody wondered when will I be able to know if I can work with other students on a project? Well, that is a question that you will meet during the work of this week. So in this week, you will be asked to fill out your choice. Do you want to work on a project or not? So no worries, that will come. The HPC access is described for people at Ghent University, but that high-performance computing system is Flemish infrastructure. That means also people from the University of Antwerp or from other Flemish universities can get access to it. If you don't know how, you have to ask this at your local responsibles for HPC. People who are volunteering students, not based in Flanders, if they want to get HPC access, that is not something we can arrange for. But you can always look around at your institution whether that is possible, if you want. Do you need HPC access for this course? No, the exercises are designed to run on a laptop. Sometimes it can be a bit demanding for your laptop, but in principle, everything can run on a laptop. HPC is a nice extra, and especially if you do the project, it can open some new possibilities. But it's not a mandatory requirement to take this course. People sometimes wonder if I use my laptop compared to the people who use a bigger machine, will my calculations be less valuable? Will they be less accurate? No, maybe they will be completed on a longer time scale. You will need more wall clock time to complete your calculation. But the result will be the same as the result obtained by people who use an HPC system. Also, somebody wondered if I want to do the project, do I have to use the Quantum Espresso DFT code? Or can I use a different DFT code? If you are familiar with a different DFT code, and you want to do the project with that code, yes. That is possible. But then you have to coordinate with the other people in your team, whether that makes sense. Maybe to verify whether two results, two calculations, if you do them with two different codes, whether they lead to the same result. That can be useful. Or when you can calculate with your code a property that is not so easily accessible by Quantum Espresso, or the other way around. So it is perfectly possible, but you have to coordinate with the other people in your team. So much for everything that was related to the practical organization. And I will go to the chat to see if there is any question. Apparently the live stream was frozen for a few seconds. Can happen. Never sure if it's only for a few seconds, never sure at which side it is. Is it the broadcast or is it at the receiving end? So I wait a little bit longer to see if there are any further questions on the practical aspects. Before we move on. To the science of the past week. I don't see anything appearing now. I will get back to the chat. So if you still think about questions, you can still put them there. I will come back to it. Then we move to the science. The first thing we did was looking at this now rather old but still relevant presentation of Gerbrand Sieder in 2014, I think, about the creation of materials from thought. And in the RE1 board file, I asked you to rate how confident you are about the statement. I can explain why. Why the vision of materials design at the quantum level is

attractive for a material scientist. And you see that many people are towards the rather confident end. So that means that you can, to some extent, explain this. Or at least you feel confident that you can explain this. If I look through your answers, I see that many people agree with the vision that Sieder had sketched there. And if I compare that to what I remember from, say, five to ten years ago, this strong agreement is really a change in attitude. Ten years ago, many people were very reluctant to accept this vision. Now the mood has changed. Not surprisingly, because now there are many more examples where a computational approach to material science problems has turned out to be successful. Ten years ago, this was much more controversial. And I quote here a few of the statements you wrote about, from people who agreed with this. I'm quite excited about this vision. Not totally 100% experiment-free yet, but we are heading in this direction. Or, in a different way, if you can do materials research by computation, why would you still do experiments? These are enthusiastic reactions. But several people also put a word of caution. And often, well, this is one of the ways how to formulate it, these methods are becoming more and more realistic, but they are never 100% exact, and we will still need experiments to confirm the predictions made by these calculations. And that is very much true. It's not because we can do many things by computation nowadays that experiments will become totally irrelevant. At least not. They will not yet become totally irrelevant in the foreseeable future. What it will be in a century from now, that's, again, that's a totally different matter. There was also a comment, somebody who was very surprised to hear about how little materials we know their properties. And that's indeed something that many people are not aware of. If you think about, say, the speed of sound, well, in how many materials has the speed of sound been measured? If you would list them, that will be a marginally small fraction of all the materials that are available. For most of them, we just don't know. Probably because we just don't care. Nobody cared enough about the speed of sound in some exotic crystal, because nobody needed it. But that means that there are maybe a lot of interesting materials around that have already been created, but that are just not measured for the property that we are here concerned about. There may be hidden gems in the material space that we know of today. And computation can be a quick way to recognize such materials. Nowadays, many property databases are in the first place computed properties. And people will do the measurement only if it turns out to be an interesting prediction. If you suspect that that particular material will have a particular property that is very interesting. A few people also made the comment that this vision of designing materials by computation, that this will be even accelerated by the search of artificial intelligence. And I very much agree with that. You didn't hear the word artificial intelligence in that video by Cedar, because 10 years ago nobody was talking about it. But now this will probably be a game changer. Already now you see many examples of calculations that would not have been possible if AI wouldn't have been involved in one way or another. So that is something that will make this vision even more likely than if AI wouldn't have been there. There was a somewhat philosophical remark of somebody who questioned the title Materials from Thought. Because, according to this person, this was not really creating a material just by thinking. It's making an analysis of data. And, yeah. I agree with that. The title of this video, the title of that presentation, was probably meant to be a bit provocative. Thought was here used as the antipode of lab. You don't use experiment. You use something that is not experiment. So let's call that thinking. But it's not really like this. You don't dream a new material. You search patterns in data. And based on that you make your predictions. Which, and this was implied in this comment here, which also means pattern recognition. That is typically something that AI is very good at. So that too can be a way how AI can help in design of new materials. And another interesting comment. Somebody who wondered, you need computers, and preferably fast and

powerful computers to run these calculations. Not everybody has access to them. So aren't you restricting in this way the progress in science? To those people who have access to fast computers? And that is the case, yeah. That is true. Is that different from what happens in the lab? Not really. Because also in the lab, progress is happening in those labs where you have the most fancy equipment. Not all progress. Some labs with less fancy equipment. But with smart science, but with smart scientists, can still make breakthroughs. And in computation it will not be different. You don't need to have the fastest computer on earth. But if you have a laptop and you are smart, there is a chance that you will find a particular question where you can make progress. So although science is not democratic, money matters. You need a lab. You need computers. But your smartness matters as well. And smart people with a lot of money, for sure they have a big advantage. But smart people with less money can still do meaningful things. And this is the same for computation as well as for experiments. So let's be aware of this. But this is not something we can change in the world. We can advance science, we cannot so easily change the society that is around the science. And a last remark was somebody commenting on the role of defects. The reasoning goes like this. It's part of the answer that I didn't put here on the screen. But the example that was used was diamond. If you take a perfect diamond crystal, then that is completely transparent. But a diamond that is used in a jewel often has some color. It's pink or yellow or whatever, blue. And that color is originating in defects in the diamond. So if you want to design a blue diamond, you don't need to engineer the crystal, you need to engineer the defects. So if your calculations are limited to perfect crystals, there can be many useful properties that you will miss. That comment was meant as putting a limitation to what calculations can do. But I would say this is not a fundamental comment because we will see, even in this course, more towards the end, we can calculate the impact of defects. We can calculate properties of pure crystals, but we can also design crystals with a given defect inside. And then look at what that defect does. What is the impact on properties of the defect? That is something that in my own research is being done on a daily basis. Nobody has pure materials. There are always defects present. Sometimes they matter, sometimes they do not matter. But very often it's the defects that you need to master in order to tune the properties of the crystal. And yes, we can calculate these to some extent. OK. After this, we look at what is an ab initio calculation. It's a word that is often used. Ab initio or first principles calculations or ab initio or first principles models. What do we mean by this? And I asked you that question. Why do we call quantum physics an ab initio model? Why do we call classical mechanics an ab initio model? Is classical electromagnetism an ab initio model? What are its first principles? And I just quote here one of the possible correct answers. So classical mechanics, quantum mechanics, they are ab initio models because they start from a set of axioms, or postulates. And then you use mathematics to derive all possible observations that are determined by these axioms. The postulates of quantum physics, these are the axioms of quantum physics. Newton's laws, these are the axioms of classical mechanics. And electromagnetism, that too is an ab initio model. And their Maxwell's equations are the set of postulates that you start from. There is nobody, nothing in nature that tells you how the Lorentz force has to look like. But once you adopt, once you take it for given that this is the expression for the Lorentz force, and you start examining the mathematical consequences of this, you notice that you are making predictions that are consistent with experiments. So that postulate is consistent with nature. So that is an ab initio method. You start from a set of axioms. These are the only things you accept without questioning or proving them. And if you then apply mathematics and you predict in experiment this or that should happen, and then you do the experiment and it turns out that this is right, as long as the answer is always right, there is no reason to doubt the validity of your postulates, of your axioms.

I've put here a long comment that somebody wrote, which is an interesting one, so you can read this later, if you want. I will tell you what is in here. This person warns that we should not, well, let me start in a different way, that reductionism, the fact that you can always explain something by the underlying reason, and then again the underlying reason, and so far, further and further, until you explain the entire universe just from the behaviour of quarks, that would be the ultimate reductionism, that this is not necessarily the right approach in science, because classical mechanics, Newtonian classical mechanics, to take that as an example, that's a good ab initio method for a part of nature, but there are features of nature that are not described by classical mechanics, where the prediction of classical mechanics is wrong. Think about high-speed effects, everything where special relativity is important, classical mechanics cannot tell anything about it. Or take complexity, if you have one oxygen molecule, you can tell something about the properties of one oxygen molecule, but the concept of pressure of a gas, you cannot derive that meaning from one oxygen molecule. You need many, many, many of these molecules, and then that much bigger system can exhibit a property, pressure, that is irrelevant for a single molecule. So sometimes complexity shows emergent behavior, something new starts to happen as soon as your system gets sufficiently complex. So thinking about an ab initio method as something that you can ever refine until you have the final theory of everything, that is not useful. We have ab initio methods for different areas of science. For the areas of for the area that is everyday behavior of motion, we can describe that with classical classical mechanics. For the everyday behavior of crystals, we can use quantum physics. But for a neutron star, might be that for this very special kind of matter, our current quantum physics is not sufficient. We may need a different method there. So I am optimistic about the power of quantum physics for predicting properties of matter, but we have to be aware of the limitations. It is not the case that by quantum physics we can predict everything about everything. No. This comment serves as a reminder that we have to control our enthusiasm to some extent. Apply it only there where it makes sense. I go back to the chat to see whether there is... I see a question here. Leander asks Do you know automatically who takes this course for credits or should we register somewhere? If you are a student from Ghent University, from Antwerp, from the Enlight Network, and there is also one student from Brussels where I know about. So if you are in that group, then I know it automatically. If you are not in the categories I just mentioned, then please contact me. Good. We know that quantum physics is our ab initio method that we want to apply to solids, to crystals. And let's see what we can tell about that. So I asked you upfront if you have to define a solid, what would be your definition? And I want to make a point by that. And some of your answers were somehow escaping the point I want to make. Some people say a solid is an object that is able to keep its own structure or something that is sufficiently hard and I can touch it. These are valid definitions, well tried, but that was not what I was aiming at. I was expecting, and most of your answers proved that, I was expecting that most people will try to describe a solid as a combination of atoms. So don't read all of this. These are just a few of your answers with the word atoms or particles that was used in the same meaning as atoms, where that word is highlighted. Many people think about solids as a collection of atoms. And the point I wanted to make here is this is not the right way for us in an ab initio approach to think about this. A solid is not a collection of atoms. A solid is a collection of nuclei. In a sea of electrons, and it's the interactions between these nuclei and these electrons that generate all the properties of the crystal. We don't think about atoms, not a nucleus with some electrons as a given that then interacts with the other atoms, no. Because in a solid you can never tell where the boundary of an atom is. Only when you have isolated atoms you can deal with it that way. But as soon as you make molecules or crystals the concept of an atom in a quantum picture loses its meaning. We

still use that colloquially, but what we really mean is we have nuclei and electrons. And because these are light particles they will not move according to the laws of classical mechanics. They will move according to the laws of quantum physics. So our complete definition of a solid is a system with two types of particles positive nuclei and negative electrons that interact with each other electromagnetically and they move according to the laws of motion given by quantum physics. That will be our picture of a solid. And every year people wonder but doesn't that apply to a liquid as well? And the answer is yes, that would be the definition of that statement would be valid for a liquid as well. The only difference is that for a liquid the position of these nuclei is time dependent. In a solid, we take phonons into account that nucleus will vibrate around an average position but in a liquid that nucleus will travel throughout the entire system. So if you have a time dependent simulation then you can study a liquid something called molecular dynamics which can be quantum physics but in a time dependent way. We will not do that in this course we will stick to static calculations and that means we will stick to crystals. But you can in principle do the same for liquids. Good, we know that we want to try to predict all properties of a crystal by quantum physics. Why is that difficult? Why don't we just do that? And I asked you that question you gave some answers and let's look through them. One possible answer could be well, quantum mechanics is a hard subject and difficult to understand so therefore we don't use it. I don't agree with that because there are many things difficult and hard to understand but if a few people understand it and they write a computer program for it then everybody else can at least use that. And for quantum physics no, that is not yet happening that way. So there must be something else it's not because it is hard and not intuitive. Another answer was well this answer uses the words exchange and correlation we will see in the next two weeks what exactly we mean by this here but these are properties that are often approximated in practical calculations. So the argument that this person here develops is we have to make approximations there are things in nature that we do not know yet and therefore our predictions are very limited we lack information about nature and I don't completely agree with that answer because we can write down the exact equations that describe the behavior of all these particles inside the solid that's the Schrödinger equation so we can write it down that's not a problem there is nothing we miss in this information what is the problem what does stop us from making exact predictions that is that solving these equations is too complicated and too time consuming we know algorithms to solve the Schrödinger equation but it would take you billions of years to run them on the current computers so in practice that solution method is then meaningless that's why we have to make approximations we have to do little tweaks to the equations to make them practically solvable it's not that we lack information no, we need to turn the equations into something that is sufficiently easy to solve and therefore our approximated answers will not be completely exact to what happens in nature and that is why our predictions are not fully exact and therefore have to be confirmed by experiment somebody suggested once we have quantum computers rather than the current classical computers then we can solve such problems as the Schrödinger equation in no time and that's right if quantum computers ever are realized at a sufficiently large scale that could be a possibility it will not happen too soon therefore for the time being with the methods that are described in this course that are much more limited than quantum computing I still think we can do useful things we should not sit down and wait until quantum computers are available but if we now try to imagine if we could do these exact calculations or almost exact calculations what are the advantages and in order to highlight the advantages I presented you with the difference between construction engineering where people want to design a bridge versus materials engineering where people want to design for instance a superconductor a superconductor that has a superconducting temperature that is above room temperature I asked

you how many attempts of the bridge are built before you build the final one how many attempts of the superconductor are made in the lab before you have the final one and the answer to that obviously was for the bridge we have one attempt you immediately build the final bridge for the superconductor look at the literature of the past century there are many many attempts of the superconducting temperature above room temperature it's getting close but we are not there yet so many attempts why is that what is the difference and the difference is I hear the bell ringing and now I am not sure whether one moment ok this was a bit embarrassing but I am alone in the building and I had to open the door I wasn't expecting that I would be disturbed here so where were we in the story I have to catch my breath I was running on the stairs so what makes that difference between construction engineering and materials engineering the fact that we have an ab initio method so for construction engineering you know all the laws of statics so you can design the bridge in the computer sorry I have to catch the regular breathing again so you can design the bridge in the computer and you can be completely sure that it will stand as designed for materials engineering if we would have an exact ab initio model we could also do that but we don't have it and therefore materials engineering is still at the face of trial and error and I have one well illustration or well a cartoon that illustrates that point that I want to share with you it's a Calvin and Hobbes cartoon that some years ago somebody who was taking this course found it and shared it I like it very much it perfectly illustrates the point and therefore I want to share it with you as well Calvin and his family are driving across a bridge and there is a sign load limit 10 tons Calvin wonders how do they know that his father has the answer which is of course not a very satisfying answer but that is what would happen if also in construction engineering that final ab initio method would not be available trial and error we then moved on to the difference between theory and computation which as the confidence statements show here was quite clear for everybody and I asked you well if predicting properties of materials by quantum physics if we call that a simulation activity rather than a theoretical activity why is that and how would you convince people who think otherwise and so first is that a simulation activity one of your answers quantum based materials calculations they use the theories that have already been developed we don't develop new theories when we do this activity or in a different way we are not inventing new equations we just use them for making calculations that is two correct ways to tell why this is a simulation activity why do many people intuitively think that doing these quantum calculations that that is theory some of your opinions because they hear the word quantum mechanics and therefore they think this is complicated this must be theory or a general attitude this is not lab work than it's theory so this was the message of this part of the module there is more than just theory versus experiment simulation has its role as well theory develops the equations simulation solves the equations perhaps by invoking a few estimations and then experiment measures the same thing in the lab this is not the end of the story however somebody wondered we hear a lot about machine learning in the context of material simulation even in the context of density functional theory that will be our workhorse method will that replace the current DFT simulations in the end and there is a good chance that something like that will happen we don't know yet exactly in which form but the field is in transformation for the time being and we could say that the point that was made in that video that you have experiment theory in the context of simulation computer experiments that picture needs to be extended connected to that we will also have a fourth pillar that is everything that involves data learning from data finding patterns in data that's what AI does that this will become or has become a separate activity from the data science so we can present it as experiment theory data science and simulation four pillars rather than three now in order to run such calculations you need hardware and therefore we spent a few very general thoughts to the development of how faster

computers are developing something that in different times in history has taken different turns I saw from the comments that not everybody liked that topic and I can understand that if you think about driving a car there are people who like driving a car in a fast way and there are people who like driving a car the way how the engine functions these are two legitimate ways to deal with cars you can be interested in the result driving fast with that car or you can also be interested in the engine and not everybody who wants to race with a car needs to be a car mechanic but you can have car mechanics that also like to drive fast so therefore not everybody who applies ab initio calculations is interested in the hardware on which these calculations are run but there are a few people who are and sometimes that particular skill is needed sometimes you need to be interested in the hardware if you want to do a particularly challenging calculation maybe making a different hardware decision to make the difference between your calculation being possible or not so therefore in general terms spending some time to hardware considerations is relevant and even if you are not totally interested in the technical details of computer hardware I think there is one point that is really important and that is the sentence that is written there the lab that doubles every year this is something that sets computational research apart from much of any other research imagine you are a microscopist so somebody who works in a lab with a sophisticated microscope and you close the door of the lab you go away do two years something else you come back you open the door of the lab again what do you find? the same microscope as two years ago if you are a computational scientist and you get out of business for two years you come back to your high performance computing system you log in what do you find? a computer that is twice as fast as two years ago so suddenly by doing nothing yourself by just waiting for the evolutions in the field the hardware evolutions in the field you can do twice as many calculations in the same time as two years ago and that happens every two years and that is happening already since the seventies so that means that the progress the kind of calculations that people can do in this field in the past ten, twenty, thirty years has dramatically changed and that explains why this type of research has become so much more important now than thirty years ago where thirty years ago you could do only highly idealized systems that were maybe academically interesting but not relevant for real crystals now you can do calculations that are about what is happening in real crystals and it is the hardware evolution that has made this possible so we cannot neglect hardware at all and because this is something that changes it is always interesting to look at what is currently at this very moment the fastest hardware the fastest computer that is available currently this is the El Capitan computing system at Lawrence Livermore National Lab in the US and this is taken from the Wikipedia page if you go there you will find some impressive numbers it is an exaflops machine it can do the number of floating points floating point calculations per second is measured at the exascale not not petascale not gigascale not megascale if you compare this with computers of even twenty years ago we will not be using this machine even the Flemish HBC is far away from this machine but it is good to know what is eventually possible and these kind of systems the ones that are now at the top of the list of fastest computers in the world in less than ten years this is what you will have at every national computing center next to the hardware you have the software so here this was not meant to give immediately a complete overview of all the software that is available in this field but just to have a first glance of what is there to show that this is a mature field of science it is not a field of science where different groups are making their own software and you don't know what exactly is in it no, it is a field where you have software with large user communities good documentation benchmarks that check the performance of one development with respect to another development a mature research environment and I can illustrate in this case there is the graphical way where you have a collection of logos of different atomistic simulation codes or a

more data-based way if you go to Wikipedia to the list of quantum software you find this long list with even summarized specific properties of each of these codes so a mature research environment that was the quick review and feedback about the topics of this week then you have been asked to start bringing this into practice we will do hands-on work in this course and the main part of this first week was to get the software installed install VirtualBox import the quantum mobile virtual machine and that gives you access to QuantumEspresso the DFT tool that we will use and that then can run on your computer or if you have access to the Flemish supercomputer you can run QuantumEspresso there as well I didn't hear many complaints or concerns so it looks like most people want to get this installed in one way or another there was some discussion on Zulip about installing this on a Mac because there is a branch of Macs for which VirtualBox is not possible the technology is too different and virtualization codes like VirtualBox they don't run on Zulip so one of you has been quite creative and found a way how to install this in a different way and you find the instructions on Zulip it's a development that I have been following in the past two years and that may become the default use in this course from next year onwards but feel free to do so it would be good to acquire some input from how it works for you in practice it's an environment that can be more graphical than the comment lines in the current virtual machine so it has a more graphical user interface although you can use it on the comment line as well if you are fine with VirtualBox and Quantum Mobile no problem you don't need to worry but if you either have problems with VirtualBox or you want to explore this other environment as well feel free to go to Zulip and to follow these instructions to set up that different environment and if you would have problems then go to Zulip and let's see whether we can have them solved in the worst case send an email but putting it to Zulip and see whether somebody can help you out that's the first thing to try ok what will we do in the week that lies ahead we will start with density functional theory we will spend two weeks to the background of density functional theory as I promised not in a mathematical way in a conceptual way so we will build step by step the ingredients that we need in order to appreciate what density functional theory is about next to that there is the build up for the project please read the description of the project make your decision whether you want to do the project or not fill out the form for this you have it in the project module and then by next week I will create the teams and from then on you can start doing the actual calculations that's it for this week I will immediately go back to the chat and see whether there are other comments there but before we do so there is one activity that will be a standard activity at the end of every week at the end of every session you have here a link to a form you can either type the url or scan the QR code and in that form you have two questions that you can answer first question what are the essential things that people surely should remember about the chapter of the past week so about everything that we discussed here in the past hour that's one and the second formulate an exam question that is something we will we will I give you five minutes for this also people who watch this as an who watch the video of this not the live stream feel free to do that at the end of the week so before the next webinar I will collect all your answers and you will find them under the video of the present week and that can be helpful while studying if you read through all the essential things that all different people quote well it is a reminder for you didn't I skip something important isn't there an insight that I missed that's one and the exam questions they can help you as a kind of test try to answer them and this is a way of training yourself to check whether you master the material if you do the exam the actual exam at the end of the term I promise I will take some of the questions that have been suggested this year and you will get them at the exam as well I also add all the questions that in previous years have been suggested so you will really have a large database of questions to train yourself so that first five minutes where you can do this I leave this screen on and if

meanwhile you have other things you want to ask or discuss put them in the chat and at the end we will go back to it okay these five minutes have passed thanks for your contributions and I look back at the chat to see whether there is something left there Simon adds that the description for using AIDA labs as it is on Zulip is just comment line that the graphical part does not load okay thanks for adding this that is on the to do list for next year to make sure that we have full descriptions how to get also the graphical part running if somebody wants to play with that and finds out how it goes then you are most welcome okay we have reached the end of this webinar unless there would be a very last question I will keep the chat on for one more minute or so and I will say already goodbye and see you next week with the first part of the DFT module bye bye