Computational Materials Physics (2024)
webinar 01 – setting the stage

Welcome to the 2024 edition of Computational Materials Physics. This is an introduction session, so there will be no science in this session, but the whole setup of the course and how this course is run will be explained, such that you know what you are up to. Let me first say in a few sentences what this course will be about, and that's very straightforward. It's about predicting properties of crystals using nothing else than the laws of quantum physics. So you could consider this as a kind of black box, well it will not be so black by the end, but a kind of box in which you give a crystal as input, and just by using quantum physics a property is produced as output. In principle every property that you can ever imagine to measure about that crystal. So if this machinery would work perfectly, then you can bypass all experiments and just produce properties of crystals computationally. That is what we will try, and although we will not be able to reach that ideal situation that I just described, you can get quite a bit along that way. We will explain this procedure not in a mathematical way, which is often done in this type of courses. No, we take another approach. It will be mainly conceptual. So we will explain the ideas behind these calculations, not necessarily the equations. And, next to that, it will also be hands-on. So everything that is told will also be illustrated with actual calculations that you can run even on your own laptop, and where you can do yourself what is described in the general theory. So that is the menu for the next 12 weeks. Thank you. A few words about the background from which I teach this course. I started with this some 30 years ago, when I was doing a PhD in experimental physics, and I stumbled upon a property that I would really need to explain the material I was working with, but there was no way to measure it. That was the time, the middle of the 90s, when density functional theory codes appeared on the academic market. And I turned to one of these codes to try to calculate that property that I couldn't measure. And it turned out that I found that so much more fun than doing the experiments in the lab. So I kind of changed my topic and dealt with calculations from then on. But always with the idea, where are the problems? Where are experimental people or people in industry that could be interested in the properties that I calculate? And how can these calculations help people in experiment or industry? And because I then often had to explain to these people what were the principles behind the methods that I was offering to them? Well, that's how step by step the explanations that are used in this course evolved. Then it's time to look at who you are. So I know a few things about the people who on average take this course. There are usually a set of four credit students, either from Ghent University or the University of Antwerp, the two universities where this course is on the official program, sometimes also from other universities in Flanders. Or in Belgium, or from elsewhere, people who get the permission from their university to take this course as a four credit online course. I have to add here for the people from Ghent University who are in the chemistry department. If one of these students would see this video, I have to emphasize for them that chemistry students will deal only with part of the course. That sometimes. There will be separate webinars for the chemistry students and that the exam is different. And there will be for the chemistry students a project with oral defense of the project on the exam. But information about that for the chemistry students will be given in their dedicated course. So next to these four credit students, there are also international volunteering students that can be from everywhere in the world. I don't know how many of them there will be this year. I didn't make a real advertisement this year. We have had years with up to 100 students who really took the course from the beginning to the end. So this year it probably will be smaller. That depends to some extent on the advertising. But I expect that also this year a few international students will be able to participate. I don't know how many of them there will be this year. But I expect that also this year a few international volunteers will participate. And as this is an online course, this is easily possible. Maybe some of you have already written something in the YouTube chat about their background. I don't see anything. I expect from the numbers that the most people that are present now will be from Ghent or Antwerp. I don't see anything. I expect from the

numbers that the most people that are present now will be from Ghent or Antwerp. I don't see anything. I expect from the numbers that the most people that are present now will be from Ghent or Antwerp. Maybe from the numbers that are present now will be from Ghent or Antwerp. Any questions? Okay. Well, practically, how is the course setup? You will probably know that the main website is www.comtmatvies.org. The one that you see here on the screen. And if you visit that website you will see this kind of tile menu that has all ingredients of the course. Behind every tile there is a series of videos. and tasks that are related to the videos. The goal is that you watch these videos yourself, you solve the tasks that are connected to them, you submit your answers to the tasks, and then, sorry, yeah, you submit your answers to the tasks, and also to the specific tasks that are in the let's play section, that is the hands-on work where you have to use your own DFT code. So also, these calculations, the results of these calculations are submitted, and you can see here an example how this would look like, and this is, at the right hand side, the topic of week 4, that is about crystallography. At the end of the explanations and tasks for that week, there is a link in the description. There is a link to the let's play section. If you then, the left hand menu, look in the let's play section, there are two topics for the crystallography week, where you can do something on your own computer, that is, that has been explained in the theory section before. When all that is done, the tasks connected to the videos and the hands-on exercises, you have submitted everything. And then the next week, there is a feedback webinar, that will always be on Mondays, local time at 1 o'clock, online. In UTC, that's 11 o'clock, until the daylight saving time ends, then it will be 12 o'clock, but easiest is to remember 1 o'clock local time, Brussels time, so there will be a discussion about the tasks that you have submitted. Or about the questions that you have asked with respect to these tasks. So no new theory, no new content, but discussions on the work that you have done. These webinar sessions, they are also recorded, and the next day, at the latest, you find them on the course website, such that if you didn't have the opportunity to watch the webinar live, you can always watch it later. Thank you. For the students of Ghent and Antwerp, if there is a need for, there can also be a Teams meeting after the webinar. So if you have specific questions that are not of interest to other people, then we can discuss them there. But if you have questions that are relevant for other people as well, well, you can just ask them in the regular way, and they will be dealt with for everybody. That's most efficient. So that is the weekly scheme. Next to that, there is also a project that's an optional project, and I will explain in a few minutes what I mean by that. This is a project that takes, well, about 10 minutes. 10 weeks, where in a small team, you can address a specific computational task, and then you report about that in the form of a short paper, and a short video. Again, this is slightly different for the chemistry students, they will have a slightly different topic, and they have to do the project, it's not optional for them, and for them there will be an oral debate. There will be an oral defense in their exam in January about the project, but again, that will be explained specifically for the chemistry students in their dedicated course. The information about the project is in the last tile, the one you see here at the bottom right. I will say something more about that in due course. So the weekly scheme. The project and the exam. In the quick start section of the course, I ask you to block already now these four dates. These are the possible dates for the exam, and the hope is that once you get your official exam schedule, that one of these dates is available for all four credit students, such that we can make an exam on one single day. Again, not relevant for the chemistry students, they have a separate exam. For everything that relates to practical info, for instance practical info related to the exam, there is one communication channel, and that's a Zulip forum. If you go to the quick start tile of the course, you will find there in the practical info session the procedure. How you can register. You can register for Zulip, and in this way you will receive the communications about all practical aspects. This is here how the Zulip forum looks like. Here it is still empty, and there is this administrative news section. If you enable email alerts for the administrative news section. Then you will get the emails for all the practical things directly in your inbox. And it's explained in the quick start tile how exactly to put that setting. What about grading? I already mentioned project and exam, how does all that fit together? Well, out of the 20 points. . . There will be 4 of them reserved for the weekly tasks. And these 4 points you have already now. So right now, 4 of your 20

points are already acquired. However if there would be a week where you do not submit the tasks for that week, then one of these points is subtracted, with a floor of 0, so you cannot get negative, if you, If there are 4 or more weeks where you do not submit, the tasks that week. You have 0 out of 4. You can still get 16 points for The , ... The exam or the project . . . So this is meant as a reward for the people, who take the effort of submitting the weekly tasks. If you do that, you get spontaneously 4 out of 20 points. . . of 20 points. The due dates for submitting these tasks they are indicated in the quick start tile the practical info you see these two green highlighted boxes here there you have the lists of due dates for all the tasks and the list of feedback webinars that is then one day later where I will discuss what you submitted. So these were four out of 20 points what about the other 16 you can do that by making an exam an exam on 16 points that exam is an open book open internet exam with an oral check so yeah you know we live in times where artificial intelligence is everywhere and the usual open internet exam that we had until a few years ago well I don't want to know how well ChatGPT can answer the exam questions I want to know how good you can answer the exam questions so therefore every question has now also a short oral check. So that's one possibility to get to 20 points that's making the exam. Another possibility is by making the project the project also has 16 points and it's up to you which of the two you choose in the second or third week of the course there will be the possibility to make that choice the project will start running from then onwards and well some people prefer the exam some people prefer the project it's really your free choice. The project information is at the bottom right tail tile okay yeah and no I don't think that today I need to say anything more about the project the project task is already available at the website so if you are curious you can have a look and see whether this is a task that will fit you or not. Let me have a look at the YouTube chat to see whether any comments appeared meanwhile no so feel free to ask any question you want directly in the chat I will every now and then go back to the chat and see whether there is something to answer. Good an online course does that mean that you are totally alone no you can find support during the work for this course and one easy way to find support is to help each other for every topic at the end of every topic there is the exit button where there are some forums to fill out and at the end of that forum you find a text like here at the right hand side. Where you have a direct link to the Zulip stream specifically for that topic. So you can post their questions that I can see and that everybody else involved in the course can see and where we can try to answer your questions. Questions that are not answered spontaneously during the week will be dealt with in the next feedback webinar. Again this is the way how the link to the Zulip platform and an impression of how it looks like so at the left hand side you have you have forums or streams like they are called in the Zulip language for every module of the course. Next to this there is also a forum that you find at the start page of the course. This is the first page of the course. This is the first page of the course. This is the first page of the course. You have the first page of the course website with an I have a question button. So if you put a question there it will open a forum where you can ask your question. Well every week I look at this list and the questions that have appeared during the week will be answered in the next feedback webinar. There is also a button at the right hand side I have a problem and that is meant for technical issues. I have a problem and that is meant for technical issues. So if there should be something happening technically with the course site, a broken link or even part of the site that is just not available, you can put a message there and this will trigger an email, this will trigger a text message to me. So if I receive such a message I drop everything and I see, I have a look what's wrong with the course site. So use this really only in case of emergency when you meet a technical problem that prevents you from continuing your work for that week. Another way to get help is if you have asked your questions in the forum and you come to the feedback webinar and I give my feedback and your question is still not answered satisfactorily, you can use the chat of YouTube during the feedback webinar or if a question, a new question pops up during the feedback webinar, you can use the YouTube chat, just as today. As I said before, people from Ghent and Antwerp, if you have specific questions or technical problems with your computer or with a high performance computer, you can use the chat. You can use the chat. You can use the chat. You can use the chat. You can use the chat. You can use the chat. Like I said to you, the

feedback webinar does Human долж青. You can always do some of the continues events, the Q & A and the feed network as a feedback webinar. You can also organize a Q & A session for anybody from the Podium on LinkedIn that were already come along in the group meeting that are not relevant for anybody else. Then we can also organize a Teams session after the feedback webinar, the hour after the feedback webinar to address the specific questions but again this are foră if your question is very very specific and of no relevance for your colleagues. you can also help each other and in a direct or in an indirect way one way in which you can help is filling out the weekly are you on board form that you find also in this exit section I ask there a few simple questions about the contents of that week and I don't ask you to answer these questions but I ask you to indicate how well you could answer that question how well you have understood that topic for instance if I read here the first question on in this example which is about the crystallography week I know what a sieve file is and I know what it is used for if you have no idea what that is you can find it in the description of this video. about then you would answer one if that is perfectly clear to you you would answer six and if everybody does that I have a quick statistical overview about which topics have been understood and which have not been understood if something is perfectly understood then no need to come back to that during the feedback webinar if there is a topic with a lot of issues then I should give special attention to that in the feedback webinar so in this way by answering this form you help to shape the content of the feedback webinar to make that as useful as possible another way to help is to fill out the time reports at the end of every section you find the link to report the time you have spent to that section there is a code specifically for that page and by looking at the statistics of these answers I can see how much time everybody spends to it and therefore I can see whether the amount of work that I give you is reasonable yet another way to help if you have suggestions how to improve this course you can always click the I have a suggestion button and this suggestion is then added to a list a list at which I look every year when I make the new version of the code of the course and I try to take into account what you suggest it you can also directly help if one of your colleagues has raised the question in either a forum in the course site or on the Zulip forum and you know the answer to that question please let me know in the comment section. Thank you for watching. give the answer, then you immediately help your colleague. So far ways to get help. A very important part of today's info session are study hints. This is for some of you perhaps the first time you work in a fully online course and the way how you address such a course, that's different from the way how you work in an in-person course. So I collected over the years a few tips that I hear from students of the previous years can really make a difference in your study efficiency for this course. One very important hint is make notes while you watch the videos. If you just watch these videos and even if you completely understand them at once, but if you don't digest that information, if you don't take notes, then this information will rapidly evaporate again. So just as in a live class, it's really important to make notes. You can easily do that in the following way. You have for every video the slides that were used in that video, they can be downloaded, you get a page like this and you can make your notes on that page, either with on paper with a pen or in a digital way as you prefer. So making notes very important. Related to that, if there is a section in the video where you make a note or where you add your own ID or you make a specific summary or a statement that helps you understanding that point better, add a timestamp. Every time when you watch the video you see the clock of the video ticking, so you can perfectly indicate this note is relevant for 2 minutes 35 seconds. Why doing that? Well, if you just make notes without timestamps, then you really have to rotten them yourself, to watching these videos multiple times. Because you see here a note, ok, what was this note referring to again? Let me look back in the video what it was about, then I will understand my note. But wait, was it there? No? A bit earlier, a bit later and before you realize it you are scrolling back and forth through the video and losing a lot of time, just to find that single sentence where your note was made for. timestamp then you can directly jump to the correct position don't hesitate to pause the video when it goes too fast for you that's one of the big advantages of watching content on a video and not in a face-to-face lecture if there is a lecturer in front of the room yeah you cannot pause that lecturer so if you need time to digest something time to note to make a note time to look

something up pause the video and do whatever you have to do much better than in a real lecture or if you want to listen to something for a second time or a third time or a seventh time perfectly possible you rewind and you watch that section again which again is something you cannot do in a live lecture or the opposite if the video is too slow for you and that might easily happen because I speak rather slowly especially the few years ago when I recorded most of these videos I was speaking even slower so it might be that this is annoyingly slow for you well you can speed up the video and adjust it to the speed that you prefer which is again something you cannot do in a live lecture apart from making notes the second very very important advice that I can give you is book time in your agenda to do the work for this course you see this course is designed for maximal flexibility apart from the weekly due date All activities can be organized at a time when it is most convenient for you. That's the advantage. But the disadvantage is, if you do not book time for that, then there will always be something that is more urgent or more interesting to do. If you are making your master thesis, your thesis advisor might come into your office and ask you to do this or that, just at the moment when you wanted to watch the series of videos. Well, technically you are available, because you have no class scheduled, but you wanted to do the work and then somebody overrules it. If you block that time in your agenda, and if you tell to your thesis advisor in advance, on that day in the afternoon, from that time to that time, I will do the work for that course, I choose to do it then. But I will not do it. I will not do it. If you want to have that time blocked for it, well, in this way you protect your time. You are sure you will have the time to do this. The alternative is that we would go back to the old scheme and have three times a week a one and a half hour meeting where that is really frozen in your agenda, that cannot be shifted. That's the alternative. So you get the freedom to do the work whenever you want, but then block yourself the time, the moments when it is most suitable for you to do that work. Don't allow other activities to overrule that. Sometimes people wonder, such a course with so many videos and weekly deadlines, isn't that a lot of work? Well, I can tell many stories. I can tell you many stories about that. And one of these is, let's look at a normal course, a traditional course, in the ideal case, what would that require from you? You see the scheme there, you have a lecture, after the lecture, in the evening at home, you revise what you have studied in that lecture. You may make some exercises. You may make some notes. You can add some questions about things you do not understand. The next week, there is another lecture, and often the lecturer will ask you, were there any questions about the previous lecture? Ah, yes, you have your notes with you. You ask the questions that you noted for the previous lecture. They are answered, and then the new lecture comes, and you revise it again, and so on, and so on. And at the end of the talk, there is a new lecture, and you revise it again, and so on, and so on. And then, in the final term, you have a few weeks to study for the exam, so you schedule a few days for the course that you were studying, and you make the exam. The ideal situation. We do not live in an ideal world, unfortunately. So in the real world, this looks more like in this scheme. You go to a lecture, and in the evening, there is a lecture. In the evening, there is something else to do, and you do not revise that lecture. You go to the next lecture. You are asked any questions about the previous lecture. Of course not. You did not look at the previous lecture, so no questions. This goes on for the entire term. Then you have to make the exam, but no problem. You have a few weeks of study time there, so you do a lot of studying there. You make the exam, you pass the exam, and the week thereafter, you have forgotten everything, because things that you cram during studying, they do not stick into your memory. So you pass the exam, but you did not gain too much long-lasting knowledge. The way how this course is made, is to prevent this from happening. And we want to achieve a situation that is much more similar to what happens in the ideal world. You study the videos, and you make the tasks first, and there is then a meeting, an online meeting, a feedback webinar, to deal with the questions you have. Once these questions are digested, you are ready to study the next topic, and again thereafter, we deal with the questions afterwards. with your questions. So in this way you spend the same amount of time to every lecture as you would have spent in the ideal world, only the order is reversed. And therefore during the term the content is already much better in your memory and you would need to study only a moderate amount of time for the exam. So is this course a lot of work? I would say more

than a course in the real world, but as much as for a course in the ideal world. And as you are supposed to deal with courses as in the ideal world, the conclusion would be no, this course does not require more time than a course should require. A second way in which I could answer the question does this course require a lot of work, is by doing some back of the envelope calculations. It's a course with six ECTS credits and that means that I can ask from you an amount of work that is equivalent to 150 to 180 hours. In 25 to 30 hours of work per ECTS credit, including everything, classes, homework, preparation of the exam, projects, doing the exam, everything should be included in that. Okay let's calculate backwards, you will need perhaps three full days to prepare for the exam, if you make an exam. So I assign these 25 hours to the exam. You will watch 15 hours of video, about the total amount of video in this course is about 10 hours, but maybe you watch a few sections twice, so to be on the safe side, 15 hours dedicated to video. And there are 11 of these feedback webinars, that take 1 hour 15 minutes at most, so let's roughly take 1 and a half hours, that's 16 and a half hours. So these hours are already dedicated. I subtract them from the 150 to 180, and what remains, is you have 8 to 10 hours per week to spend to the weekly tasks. So, not to watching the videos, that's already included, but just to make the tasks that are connected to these videos, 8 to 10 hours per week. I can guarantee you, it will often not be that much. much, but legally, for 6 ECTS credits, that is what I can ask. If you need more time than this, then you have the right to complain, then the work for the course would be over-dimensioned. As long as it remains under this limit, then we are totally fine. If you would do the project instead of the exam, then the studying for the exam will not be there, and then you have even more time, 10 to 12 hours per week, to spend both to the weekly tasks and to the project. But once again, very important, that time doesn't come for free, block that amount of time in your agenda, and use that then to do the work for this course. Ok. Another question I sometimes get is the due date for the weekly tasks, that's on Sunday morning. Doesn't that mean that I lose all my Saturdays? Many things to say to that. Why is it on Sunday morning? The feedback webinar is on Monday at noon, so that typically means that I use the Sunday to prepare that feedback webinar. So. I can't put it much later, otherwise there would not be time for me to prepare the feedback webinar. Why then not putting it on Saturday evening, rather than on Sunday morning? There are people from other time zones taking this course, and there the difference between Saturday evening and Sunday morning can be something totally different in their time zone. So therefore. It's better to put it just before the time I get up. I can't put it much later, otherwise there would not be time for me to prepare the feedback webinar. So therefore. It's better to put it just before the time I get up. Then. That's the maximum amount of time for everybody. And will you lose therefore many Saturdays? Well, no, because nobody tells you that you have to do this work on Saturday. If you book your time properly. You can have another time of the week where you do the work for this course. Good. So much for the study hints. Let me look at the YouTube chat, still no questions there. You look to be a bit shy, so don't be afraid to put questions or comments in the chat. A few words very shortly about the course site development. I consider this course as being under permanent development, although in the last few years no many major changes have been made. I always try to make sure that the material for the next week is fully ready and available. As we go through this course once every year in this way, by the end of December the course is fully revised and updated. For the people who want to study self-study. The course will be self-paced during the year, not as a 4 credit student of a Flemish university. In practice, what does that mean? The last years not too much anymore, because the course is rather stable, so no major changes have to be made. I think I can say that everything up to December is already fully available. But you have to consider that this course development is a low-budget effort, with low basically meaning zero, and a one-person project. I do this course development myself. There was a few years ago a great support from a company Deteach, they did a redesign of the course site. So what you see here is the course. I would say it is a more modern looking, more fresh course site than it was a few years ago. So that was extremely helpful. But they are not supporting this course continuously. So from now on, or from already two years ago, it is again a one-person project. So I try to do my best, but I can't do miracles, there are also other things I have to do. So I am very much listening to all

suggestions and comments you make, and I try to take them into account, but maybe not as soon as you may want them, and maybe not as thorough as you may want them. I think that's more or less what I had to say for today, so let's wrap up very specifically, for the next week. What has to be done? First of all, if you didn't do so yet, go to the quick start tile on the course site. There are several items there, read them one for one. And if there is action needed, like subscribing to the ZULUK forum, then please do that. So that's the first one. The second one. It's always good to learn something about your background. So in the second part of the quick start tile, there are some questions about you, where you can present yourself and your expectations. So please do that. The third task, that's then the scientific topic for week one, that's the tile on setting the stage. The third task, that's then the scientific topic for week one, that's the tile on setting the stage. The third task, that's then the scientific topic for week one, that's the tile on setting the stage. So go through this material, watch these videos, read the texts that are included, make the tasks that are connected to these videos and texts. And the fourth part, that's then the hands-on part for the present week, which you find in the let's play section. And that consists of two steps basically. Two steps. Two steps. Two steps. Two steps. To prepare your laptop for running the software with the computational, for running the computational software, and securing your access to the HPC infrastructure. You can, you will be able to choose whether you run the tasks on your laptop or on the HPC. Especially for the project, HPC access can be useful. of course things can go faster there and you can do bigger calculations than on your own laptops so these four things should be done by next sunday 7 a.m brussels time and you will get feedback on that next monday 1 p.m brussels time and everything that i've told here will so this session is recorded and you will get in at the very end of the quick start tile you will get the recorded version such that you can look back at this information at any time later during the term that is what i had to tell and now i will go to the next session look once more to the youtube chat whether there is anything there so last chance today for asking questions anything that is not clear or where you want to have more explanation or maybe also just an assessment on how the how the video was technically done thomas asks is it possible to start the work for week two already this week yes i should have said that if you see that you will have an a busy period in your schedule one month from now but more time available next week well try to run ahead and do the work for that week submit everything already and yeah so that's that's perfectly possible to plan the work as you want as long as you respect the weekly deadlines if somebody would say i want to do the entire course in the first two weeks i spent 100 percent of my time to it even that would be possible not for the project work of course and there you have to coordinate with the people in your team but for the for the content part of the course, that would be possible. okay no further questions I wait for five more seconds I don't see anything so then we will close here and we'll see each other again online in one week from now bye bye