feedback webinar : project review and concluding words (2022-12-12)

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Well, I always find it hard to believe at this time of the year, but yes, this is already the very last feedback webinar of this course. Time always flies so fast. And we have two items on the menu today. The review of your project work, and a few concluding words. But before starting with these, let's look at a few questions that came in the past week. Well, a few questions and one reminder. Let me start with a reminder. For those of you who are students not from Flanders or Belgium, and who did not yet do it, please fill out the feedback form for this course. I would be very much interested to hear your opinion. Let's then look at a few questions. So last week somebody asked in the context of surfaces, for instance, and defects. Why do we need supercells? Can't we just switch off periodic boundary conditions? Because then you would naturally have a surface if you switch it off in one dimension. Well, that's not so easy to do, because remember the module on electronic structure. There we introduced reciprocal space, the reciprocal lattice, and we used the k-vectors of the reciprocal lattice to label our basis functions, the plane waves. And we used the k-points inside the first Brillouin zone to label the crystal orbitals. These are the quantum numbers that appear in the band structure plots. And that reciprocal lattice exists only when you have the... Sorry, I just lost my train of thought. That reciprocal lattice exists only when you have periodic boundary conditions. So therefore switching off periodic boundary conditions means that you have to drop that entire formalism of reciprocal space, reciprocal lattice. So it's not so easy to do that. It can be done, but it's not straightforward. So for two reasons, the reciprocal lattice formalism and the plane waves as basis functions. Now there are codes who do that. This is a Wikipedia page where you have a long table with an overview of almost every quantum chemistry code that is available. And you see there in the third column, here every time when there is 3D it means you have periodic boundary conditions. And these are the names of the codes. And the basis functions they use are very often our plane waves. So 3D periodic boundary conditions and plane waves, they go together. If you go deeper in that list, you will find other codes with Gaussian-type orbitals often, numerical atomic orbitals. They can have either periodic boundary conditions or no periodic boundary conditions. And even deeper down in the list, in this part, you have codes that have no periodic boundary conditions, so where you can only do molecules, clusters, and these are all with Gaussian-type orbitals, so with local orbitals. So if you have a local orbital code where you put a basis function on the position of every atom, then you can switch off periodic boundary conditions. If you don't, you can still keep the k-point formalism, that's not impossible, but it's mixing the languages of two worlds. A second question that arrived a few hours after the previous webinar, you don't have to read everything, but it's interesting to see that people really digest these webinars and spot places with exact time stamps where things are not clear. So it was about this slide in the previous webinar, where I very quickly, under some time pressure, told that this is the potential in a slab, and by the energy difference of an electron that is inside the slab and outside the slab, you can determine the work function. And somebody noted, well, that explanation is a bit different from what is given in the course site. There it is told that you have to take the energy difference between the potential outside the slab and the Fermi energy, not the potential inside the slab. And that is of course the correct statement. I was a bit sloppy here in quickly telling that story. You need the energy difference between the electron with the highest possible energy inside the crystal, and that is the Fermi energy, that is how the Fermi energy is defined. That energy, and the energy outside the slab, when it is fully in the vacuum. That energy difference is the work function. So yes, the Fermi energy is the object you have to look at. And another question, somebody who looked at the density of states calculation for the silicon crystal, and computed the integral of the density of states, which we said that is the number of electrons in the unit cell. And this person found, well, if I do this, I find 8.76, and I would expect for silicon, it has 14 electrons, there are two atoms in the unit cell, so I would expect 28. Why do I find that strange number? Well, what can we say about that? Look where silicon is in the periodic table. So in the p-block, we have the density of states, that is just a picture taken from the web, but you calculated something very similar. Here the valence band is colored, and if you would integrate that, you will not find 28, you will find 8 exactly. Why 8? Because this is only the region of the energy region where the valence electrons are, which for silicon are the four outer electrons, the 3s and 3p electrons, two 3s electrons, two 3p electrons, so four of them, and they are in that energy range under the Fermi energy, and therefore the density of states would have twice four electrons, so exactly 8. Not this 8.76 that this person noted, I didn't check where that number came from. Maybe, because you need quite a precise integration to get the exact number, maybe that was just done on a rough grid, but if you do it correctly, you would find 8. Where are the other 20 electrons? Because they do not disappear. If you would extend this picture, if you would look deeper in energy, you would find way, way, way, because this picture is not on scale, so you would find a few meters to the left-hand side of the screen, you would find very sharp peaks with the 6 2p electrons, if you would integrate that peak on a very, very narrow grid, you would find 6 2p electrons times 2, so 12. You would find a peak with twice 2 2s electrons and twice 2 1s electrons. Numerically they are not there, because you have the pseudo-potential for these electrons, so they do not exist for your calculation. But physically, if you would do this with an all-electron code, you would find there these very sharp peaks. The physics is correct, but we make numerical tricks to deal with this. And we are not interested in these very deep core electrons, because they do not participate in chemical bonding, so they are just spectators of the problem. Therefore, we never plot them. That were the questions that arrived. Let's now look, or maybe let's first check the chat, whether there is anything, no. Let's then look at your project results. Always a very interesting journey to look what you have found in the past weeks. Oops, see I was in a hurry this morning, there are slides there that should not be there. So there were different topics for the project, and let's do them systematically. The first topic that has been dealt with by two teams, was the iron-silicon problem. And especially for the ones who did not work on this, so what was the story about? We have a phase diagram, with at the left hand side pure BCC iron, and at the right hand side of our phase diagram, we take an alloy with, for every three iron atoms, there is one silicon atom. In this particular crystal structure, that is a unit cell, so the blue silicon atoms form a kind of tetrahedron, and all atoms are at positions that if you would forget the elements, if you would forget the colors, this would be a BCC lattice. Now such iron-silicon alloys are useful as electrical steels, you will use them as the core material of transformers for instance, or in electrical motors, and therefore you need to have a material with the right magnetic properties. What is right is not something we are concerned here about, but engineers have found that if you have a silicon concentration that is about half between the iron case and the iron-3-silicon case, then you would have an alloy with the ideal magnetic properties. However, in real transformers, in real electrical motors, you will not use a material with this concentration of silicon, you will use one with this concentration, which is not ideal. Why do engineers do that? Because if you would increase the silicon concentration more, the material would become brittle. So you can't machine it, you can't produce anything in a useful shape out of it. So we are forced to use a suboptimal iron-silicon alloy. The goal of this project was, let's try to understand this brittleness. Can we find ordered phases in the phase diagram of iron-silicon around that concentration, and if they are there, that could be the reason why this material tries to order itself, and once a material has long-range order, then it is more brittle than if it is a more random alloy. So let's hunt for maybe existing or maybe not existing ordered phases in the iron-silicon phase diagram. And there are two teams who have dealt with this, the team by Arthur, Cedric and Corentin, and the team by Jason, Nidi and Hijaz. I hope I pronounce all these names more or less correctly. Forgive me if that is not the case. The first the teams did was convergence testing. We learned that this is the good practice, and team one suggests two sets of parameters, one for medium precision, one for high precision. Team two settles down on one set for good precision, and so if you compare all of these, you see that convergence testing is not a straightforward procedure. It depends on your appreciation to some extent. What you conclude is a well-converged setting, or which one is not. So team two goes to a basis set size of 140 Rydberg, which is even larger than the high precision setting of team one. I don't say which one is best here, that really depends on the criteria you use, but it is just a reminder that this is not a question with one single unique answer. The second step was geometry optimized, the two endpoints of the phase diagram, the pure BCC iron and the iron III silicon. And what we learn here is that units matter if we want to compare. So this arrived 24 hours ago, so I didn't look at all the details, I didn't make the conversion, so I guess looking at the final results, that both answers are correct, but one answer here is in Rydberg, the other is in electron volt per atom, the volume is in cubic Bohr, here the volume is in cubic Angstrom, so you can't verify just by first sight whether these values are the same or not. But both teams found an optimized geometry for these crystals. Interestingly, team 1 also kept track of the magnetic moment per formula unit or per unit cell, and so that is one of these useful properties that the engineers for the electric motors will need to use. Team 2 on the other hand, also calculated the bulk modulus for instance for the two materials, so you can already see that the iron III silicon has a higher bulk modulus than BCC iron, so intrinsically iron III silicon will be harder and therefore more likely to be brittle than BCC iron. The third step was what we called a sanity check. I gave you one crystal, one alloy, in that range and calculate the formation energy of that alloy. And you see the alloy on the screen, so at the left hand side is the pure iron III silicon, and the silicon atom that is indicated is replaced by an iron atom, so you move a bit to the left on the concentration axis. You are at three quarters of the distance between iron and iron III silicon. And from here on you can measure this with a variable x, x0 is BCC iron, x1 is iron III silicon, and x from 0 to 1 indicates any alloy in between. You can use that x to calculate the formation energy. If you have expressed all energies in energy per atom, then you take the energy per atom in the crystal you are studying, minus x times the energy per atom in the DO3 crystal, minus 1 minus x times the energy per atom in the BCC crystal.

And both teams find a value which is very slightly positive, around 0.01 electron volt per atom. Positive, that means it takes energy to create that alloy out of the two end alloys. So that alloy will not form spontaneously. Again, I didn't verify whether this is numerically correct or not, but the fact that two teams find nearly the same number is reassuring. On the other hand I must say I have given the same task to the chemistry students, and there three teams found a value that was considerably negative. So this afternoon or tomorrow I will verify the two sets of numbers to see what can be the reason for that. Then what was it really about? Searching other alloys that are somewhere in that range and that maybe have a negative formation energy. And team 1 first made an analysis what would be the interesting alloys. So if we have a number of N atoms in the unit cell, how many silicon atoms do we need in that unit cell in order to have that ideal concentration? That is 12.5 atomic percent or about 6.7 weight percent. That turns out for a 16 atom cell you need two silicon atoms, so even one less than the one we just used as a test case, for a 120 atom cell you need 16. And you can imagine if you have two atoms out of 16, then you have a limited number of combinations how you can put these two atoms. If you have 16 for 128 you have many more combinations. So this is a combinatorial problem, if you want to really examine all possibilities that will rapidly grow with the size of the unit cell. But nature has infinite unit cells, so nature has infinite amounts of time to find what is the optimal configuration. Let's see whether we can find some of these. I continue with team 1 for the time being. So they looked at cells with 16, 32 or 54 atoms and made three cases for the cell with 16 atoms, eight cases for the cell with 32, four cases for the cell with 54. And I think if there was an X there, it means they could converge that calculation. If there is a question mark, it's not converged. And I show on the picture two of these cells with 54 atoms, where you can recognize that this is a 3x3x3 BCC iron cell, with in this case five of these 54 atoms replaced by silicon, and that forms a kind of large tetrahedron with an atom in the center. And in this case you have six silicon atoms and they form kind of diagonal lines through the crystal. Now, team 1 reports that a few of these cases are close to zero information energy. There was not a number because probably they did not succeed to fully converge everything to do the full geometry optimization, but it came close to zero. Which is an indication that there might be something, even with this limited set of how many, 14 different cases, you find already some that are close to being stable. Interesting. Team 2 did a similar game. Their tree looks like this. And the pictures here are shown without periodic boundary conditions. So every atom that you see there, you can count as one atom in the unit cell, and you recognize here the tetrahedron of silicon atoms, so this is the full DO3 crystal. If one of these atoms is replaced by iron again, you have the test case, and then the other ones were different combinations of having just two silicon atoms. Now here is one silicon atom, and the other ones are two silicon atoms, in different relative configurations. You can put that on a phase diagram, and that is what they get. So this is from X0 to X1, or in atomic percent from 0 to 25. This was the test case, with this formation energy of about 0.01 electron volt per atom. If you have only one silicon atom, the formation energy is still positive, but closer to zero. The other cases with two silicon atoms, they are here, so they are less favorable than one or three silicon atoms. Team 2 went one step further, and also looked at a larger supercell, so a 2x1x1 supercell, where you have two of these DO3 cubes next to each other, and if that would be just DO3, that would be the left hand side picture. Now they replace in that structure some silicons by iron again, and they take the interesting concentration, so four silicon atoms in this 32 atom cell, and there is a kind of line of silicon atoms that is running diagonally here, and another line that is diagonally, let me try to do this with my arms, this way, a line of silicon atoms that is going this way, and another line of silicon atoms that is under an angle of 90 degrees with the same one. So I turn it 45 degrees for you. This is how the silicon atoms run, but separated from each other by one, two layers of iron. What does that crystal do? It has an energy that is still positive, but really close to zero. So just as for team 1, again an indication, there is something there, and if we play more, then maybe we will find something that drops under zero. Team 1 also constructed the input for the cell that I suggested in the beginning, as a possible interesting candidate, without realizing at that moment that the computing time would go up that quickly. I didn't do any tests here, so I was just hoping that this would be doable, but for the scope of this project that was a bit too much, but still the input was constructed, and I called this in the project description a kind of fractal structure, because you have the same pattern repeating at different scales. The DO3 had this tetrahedron of silicon atoms, and now we take a 2x2x2 cell of the DO3, and we put that tetrahedron in a tetrahedron shape. So we put one here, one here, and then one here and one here. So four out of the eight cubes have the silicon atoms, and these four cubes form a tetrahedron in the larger supercell. The concentration is the right target concentration, and I have some suspicion that this would be a particularly stable crystal. We could not verify this, but the input is there, so now it is just a matter of letting this run for a while. That was the iron-silicon topic on which two teams have worked. Team 4 was a team from the University of Basel, a chemistry group there, and these people suggested their own topic, and worked on that one. So Dietger and Eyemal, and that was also a very interesting one. They are studying clusters, so they are a bit bothered by periodic boundary conditions. Their natural world is clusters, molecules, so they have to work in a supercell with just one cluster. But their clusters, they tend to bind to other clusters and form superstructures, so it is not too bad of an approximation to take a unit cell that contains just one cluster, and not too much vacuum, that allows it to bind to the periodic copies, and that is a good model for nature. Which type of clusters? Look first at the right-hand side. They have six metal atoms, the ones that are in light blue, bound with eight oxygens, the ones in red, and then the bridges between oxygen and the metal, these are decorated by organic molecules, so that you see on the left-hand side. And that picture on the left-hand side looks from the top of the picture on the right-hand side, so it is not just a copy one of another. These look to be many atoms, but most of them are relatively light atoms, so not many electrons, and with the computer they used that was a doable calculation. So the question they asked was, if we know we can make in the lab clusters with one metal, and clusters with another metal, but what would happen if we try to make clusters with two metals, so that some of these six metal atoms are of one type, and some of the other type. Would these clusters be more or less stable than the end members? That is in a way a very similar problem to the iron-silicon problem, it is a kind of phase diagram, and we have to see what can be formed, what is stable in that phase diagram. They did the convergence testing for the k-mesh, the basis set size, and the factor for the basis set for the density, and they did that for three different clusters, with three different metals, zirconium oxygen clusters, hafnium oxygen clusters, and cerium oxygen clusters. And they make a phase diagram out of that, so you can read this picture really as a phase diagram, the zirconium oxygen cluster at the left, with an energy that we take as zero, just as for iron-silicon, we normalize it to zero here, and we normalize it to zero at the other side, at the hafnium cluster. And now all clusters that can be made in between, for the different zirconium to hafnium ratios, and for some ratios, like if you have two hafnium atoms and four zirconiums, there are different ways in which you can position these on the six available sites. So they did all these combinations, and these are the formation energies they found. Now it's not written in their report, but one interesting thing you can immediately do with this is, let's really consider this as a phase diagram, and make a convex hull construction. So I put the convex hull here, and what do we learn from this? There are three mixed crystals on the convex hull. This one here, the 3-3, which is lowest in energy, this one with two hafniums, the convex hull line just goes through it, so it's not likely that this one will form, because it can split into these two end members at the same energy. So that will probably be some dynamic equilibrium. And the one with one zirconium and five hafniums, this one is on the convex hull too. All the others, even the ones that are the examples here, this one here has a negative formation energy, mixing the two pure clusters will lower the energy, but there is another one that is even lower. So only these three are the ones that are candidates to form. They did that with zirconium and cerium as well, same game, the convex hull is now much simpler, only one of them, the lowest energy cluster, is a stable one. Everything else is above the convex hull. So here it's even more dramatic, you can take this 3-3 cluster, it has a strongly negative formation energy, it is the lowest energy of all the possible arrangements for these 3 plus 3 atoms, but nevertheless it cannot form, because you can gain energy, or you can even lower the energy, by splitting it into a pure zirconium cluster and a zirconium-2-cerium-4 cluster. The fact that this picture is different from the zirconium-hafnium picture is already interesting. It shows that there is rich chemistry happening here. It's not sufficient to do this once for one mixture, and then immediately you know which clusters are potential candidates, no, you have to do it for every case individually. The last case they did was with hafnium and cerium, so they have all combinations for cerium, hafnium and zirconium, and here the convex hull looks like this. So three times different behavior. They even tried to make clusters with three metals, and these are the ones with mixed zirconium, cerium and hafnium, these are the ones they tried. They did not do that in their report, to analyze it that way, but what you would need to do here is to make a phase diagram in three dimensions, and then again make a convex hull construction, but in three dimensions. And that would tell you which are the stable phases in these three metallic clusters. So really a rich topic where interesting information can be found. Team V, there was no report for Team V, but I want to specially mention Timo, because with not much time available and being alone, he did nice tries on hydrogen storage materials. The time of the resources he had was not sufficient to complete that, to something that could be reported, but it was, from what I saw along the way, it was an interesting study, and something that has the potential to continue to work on. And Team VI, Jyoti from India, she studied the other topic that was suggested in the beginning of the course, the FCC aluminum crystal, where we were interested in how unique is the DFT answer. If you calculate the total energy for FCC aluminum, we normally take the primitive or the conventional unit cell, but how much does that computed energy depend on that choice of unit cell? Because even the primitive cell, that's one of the infinite number of choices you can make. You can make an infinite number of cells that have exactly one aluminum atom in the cell, and that construct the FCC lattice. Is our code numerically robust enough to give every time the same total energy? Or, if that is not the case, what is the spread on total energies? And what is therefore the numerical error bar on your total energy? This is not something that, as far as I know, has ever been really examined. We just take it for granted that we work with the primitive or the conventional unit cell. But, well, let's test that. So, what was done here, a convergence testing for the normal primitive FCC aluminum cell, and the values that were found, the k-mesh was quite dense, because we really need high precision calculations here. We have to be prepared to see differences in the six digits, maybe. So, let's do it precisely. Geometry optimize this, because we want to have the lowest energy cell, and then we will start making different choices of that cell, but with the same volume per atom. So, the energy versus volume calculation was done, the minimal energy was found, the equilibrium volume, the Bolt modulus, a direct application of the geometry optimization topic. And then we can start making different cells. So, I show here some of the plots from the report with different cells. The table has the a, b, and c lattice parameters of these different cells, and the angles, and the energies. And at first it is quite shocking to see how different these energies are. I see their values, 39.502, that's what you would expect, that's what the regular primitive cell gives you, and there are their values that are even 21 Rydberg, so 18 Rydberg different, that's impossible, cannot be. Then if you look more closely at the pictures, I see that, for instance, all these angles here are either 90 or 60 or 120, and let's take the case number 8, the last line, which is this picture, picture 8, I see here angles 90, 90, 90, but that is clearly not what is happening in this picture. This is not an orthorhombic cell, there is an angle of 120 degrees there. So that makes me suspicious that something went wrong in the construction of these unit cells. So probably these numbers are just not right, because cells have been taken that are not what they are meant to be. But the idea, the workflow of how this is tackled is correct, so if the goal was to find a number of primitive cells that are not the default choice, calculate the total energy, so that has been done, but unfortunately the choice of cell, the construction of these cells, has probably not been done in the right way. Nevertheless, really an interesting exercise, and also that one is worth looking at more closely. Well, that were the reports that were submitted, so I certainly must congratulate all the teams. I know this is a lot of work, and especially the last two weeks probably that goes into a crescendo mode, but the work has been done now, so you can relax. There is one small extra thing to do for the teams, and that is to do your team introspection. So in the coming week, with the usual due date of Sunday morning, go to the module on the project. The last item, there is a self-assessment and team introspection forum, that everybody should fill out for himself or herself, where you evaluate how your team has functioned, how your teammates have functioned, how you have functioned in the team, and I will then combine this information, and you will never know what your teammates have told about you, but I will see it, and I can see whether this is an honest assessment of everybody's collaboration, contribution to the team. So that is one thing. The other thing is, probably from tomorrow onwards, on the previous item here, the gallery of project results, you will see the four papers that have been submitted, with the four videos that the teams have made, and you will get personally an email indicating which two of these videos and papers you are asked to read, and to give your comments on. So a kind of peer assessment. You have done such project work yourself, so you are in a good position to say something meaningful about the projects of other teams. And these peer assessments, they will be taken into consideration for the grading, because the people who did the project, they don't have an exam, they will be graded on that project work. And it's not that the other teams will grade you, no, they will give me some extra input to fine-tune my grading. And when that is done, then all the work for this course, for the people who did the project, is completely finished. Let's see whether there is any question or comment on this. Any project-related comment or consideration? No. Then let's have some concluding words, practical and non-practical. So, a last time, the ones not from Belgium, who did not fill out the feedback form yet, please do so. The ones who didn't do the project and who will do the exam, so the four credit students, what if they have questions? I told that last week, but I repeat it here. You can send a question still in the usual way by clicking on the I have a question button, but as the exam is approaching, preferably also send a copy of that question by email, then I'm sure that I will see it and then I can answer you also personally. If there is a question of more general interest, I will include them in the Frequently Asked Questions section. Then others can read it as well. That Frequently Asked Questions section is the very last module of the matrix on the first page of the course. Then the scientific concluding words, and this is a story, I tell it every year, and I could have told it at the beginning of the course, but I deliberately didn't tell it there, because I expect that now it is more meaningful to you. It's a story that goes back to my youth. I had a good relation with my grandfather, and my grandfather often asked me, what did you learn at school? He was very interested in what I did at school. And one day I told him, today we learned in the mathematics course about square roots. My grandfather was very interested, square roots, and how did you learn to calculate them? And I didn't know exactly what he meant by that. How did I learn to calculate the square root? There is a button on my pocket calculator, and if you press that, you get the square root. So that's what I told my grandfather, and he was upset. He said, no, that cannot be. In that way you do not know about square roots. You should calculate them by pen and paper. There is a procedure for that. And he taught me that procedure, and that was interesting, and I was happy that I could calculate square roots by pen and paper. I forgot meanwhile how to do it, but you can find this on the internet. There are recipes that look very much like a long division, but with different rules, and if you go through that procedure, you find the square root. Now, I tell that story because it shows the difference between the concept of something, the concept of a square root, because that was what I learned at school. I learned what a square root is, and the numerical work that we give to the pocket calculator. While my grandfather, who lived in a time without pocket calculators, he learned the procedure. And in his mind, the concept and the procedure were one. You cannot know about square roots if you don't know how to calculate them. That is an attitude that has been in the field of DFT for a very long time. The people who, in the 80s and the 90s, developed the codes that we are now using, their approach was, doing DFT means you know the procedures, you know what all these subroutines are doing, you know the algorithms that the code is internally using. If you are just a user, as they call it, the one who presses the button and gets the total energy out, then you don't know what DFT is. That attitude, so around the year 2000, was quite strong in this community. And I never agreed with that attitude. And this course is made as a reaction to that attitude. An attitude that is now not that strong anymore. It is now generally accepted that you can do DFT in a meaningful way without being a code developer. You don't have to know all the recipes that happen internally, but you need to know the concepts of DFT. You need to know what you are doing, and how it is done, that we give to the DFT code. So that was the mindset of this course. And therefore, we learned conceptually what DFT is, and we learned some practical tricks to make sure that we do meaningful calculations. What is the convergence testing? What precision can you expect? What accuracy can you expect? These are practical and theoretical conceptual visions on DFT. Then we had a look at how do you give input to your DFT code. So we need some crystallography, because we need to understand the unit cell that we give to the code. And as an elaboration on that, we can also do less perfect crystals, we can do surfaces, we can do defects if we have supercells. Once we had given that input, let's allow the theory to find the most optimal version of that input. So let's geometry optimize our input, and that led us to phase diagrams in the end. Based on the total energy, and the optimization process can also use gradients of the total energy, the forces. Once you have the optimized unit cell, so the prediction of DFT for that particular crystal, you can analyze it deeper with the language of physics. You can look at the electronic structure, which is the basis for many spectroscopies that we didn't look at this course, but this is a very big field, theoretical spectroscopy. We looked with the language of chemistry to understanding chemical bonds in our crystal, with the charge density difference plots for instance. We looked with the language of engineering to elasticity. We computed some of the elastic moduli that engineers love to use. All of that for perfect crystals, and you could also apply this for crystals with defects or for surfaces. So that was the practical, pragmatic way in which we tackled DFT. And that is how I hope we have made the step from knowing a procedure, to understanding a procedure and applying it thanks to a tool, which is our pocket calculator, here our quantum espresso or other DFT codes. And I hope by having learned all these things, that you are able to read papers about DFT, because whatever research you do, you will find people who in your field of research publish DFT based results. So with the knowledge of this course, you can understand what they have done. And if you see they even don't mention how they did the convergence testing, then you can put that paper aside and there is no need to trust it. So you can be critical towards what these people, but otherwise you use magical tools, what they would try to tell you. They have to do their job right before you should believe them. And that was my really last word, so I have nothing more to say. I stop here and I just wait for a few minutes more, in the chat or in the room, last questions or comments or thoughts. Yes? When is the exam? As far as I heard, so the question is when is the exam? As far as I heard it will be the 19th of January, but that information has not yet been officially communicated, I thought, to the students. Did you receive your exam schedules already? Officially? If it has not yet been communicated, it will be communicated this week and the last thing I heard was it is the 19th of January. But I don't think that I am allowed to tell this. It will be recorded, so I am breaking the rules maybe, but... Okay, no further questions, so we can stop here and no next time anymore. See you later.