A trial version of an on-line course on computational materials physics is starting soon -- volunteering participants are being searched.

DFT is no longer a tool of only the theoretical physics and chemistry communities. Knowing how to interpret papers with DFT-results, and/or being able to make basic DFT-calculations in a responsible way, have become relevant skills for many scientists and engineers. In response to this evolution, many universities around the world offer courses that introduce students to the interpretation and application of DFT.

Given the general need for such a course, it makes sense to think about an on-line format to deliver one. At Ghent University, we've been playing recently with low-budget ways to deliver courses to an on-line audience (low-budget means: limited costs for the instructors, no costs for the students).

The course "computational materials physics" -- offered locally to students in materials science, physics and engineering physics -- is now in a shape that makes it suitable to test on a larger on-line audience. **If you know volunteering students who are interested to participate, please give them this information.** If you want to inspect this course as an observer without active participation, this is possible too. Perhaps you may want to give constructive comments, or even contribute material for future editions. The course starts on September 26, and runs until mid December. Every week, students receive a set of video material and a set of tasks. Answers to the tasks have to be submitted on a weekly basis. There is a weekly class session, in which problems and questions students met while solving the tasks will be discussed. The class session will be live-streamed for on-line participants, and a recording of the class session remains available for one week. Actively participating students will be asked to team up to work on a project throughout the course. In the last session, project results will be presented to the group. DFT exercises will be made using Quantum Espresso and the Virtual NanoLab interface, although you can use your own favourite DFT code if you want.

Don't expect very fancy material. The bottom line of this endeavour is to create a fair on-line course, without investing an excessive amount of time, and at very low cost. It should be fair, it should be interesting. Nothing more.

The target audience is in the first place people who have no prior exposure to DFT, and who want to acquire a basic knowledge (including basic hands-on knowledge). Emphasis will be on conceptual understanding, and on practical work. The course is not meant for experienced DFT users or for hard-core theoreticians.

You may inspect the course site at <u>http://www.compmatphys.org</u>. Mind that the site is not yet complete (more material will be added as the course proceeds) and that some available pages are still under construction (those will be ready when the course starts in two weeks). Some pages can be accessed without signing in. If you sign in, you can see most of the material. Signing in does not bind you to anything (you will be signed out anyway if you are not active on the site for some time).

Participating in the course means you should be ready to invest 3-6 hours of work per week, during 12 weeks. Participation is on an entirely volunteering basis: there will be no exam nor any official or legal certificate.

If you are interested to participate in this course, as a volunteering student or as an observer, please fill out this form: <u>https://goo.gl/forms/8n5SqKZqoCV2CRM63</u>. As this is a test phase, we cannot accept yet an unlimited number of participants. You will be informed whether or not your participation/observation is accepted. Preference will be given to people who are willing to participate actively, and to observers who are willing to give constructive comments or who consider contributing material for later editions. Depending on the outcome of this try-out, we will consider whether or not to offer this course on a yearly basis. If people from the Psi-k community are willing to collaborate on this, please contact me. Together, we can definitely make it better.

Stefaan Cottenier

--Stefaan Cottenier Center for Molecular Modeling (CMM) & Department of Materials Science and Engineering (DMSE) Ghent University Tech Lane Ghent Science Park – Campus A building 903 BE-9052 Zwijnaarde Belgium

http://molmod.ugent.be http://www.ugent.be/ea/dmse/en email: <u>stefaan.cottenier@ugent.be</u> my conference talks on Youtube: <u>http://go</u>