Lecture "Advanced Material Modeling"
Skolkovo Institute of Science and Technology
Description of the "Advanced materials properties" lab (lab #1)

A. Objectives

In the "Basic Materials modeling" lecture, the students have been initiated to the usage of several modeling software applications, for molecules and for solids. In particular, as concern the modeling of materials, they have learned how to use VASP (among others) for the computation of basic properties of crystalline solids, namely total energy and lattice parameters. VASP is one of the most used software application for the first-principles computation of condensed matter properties.

In the "Advanced Material Modeling" lecture, one of the goals is to allow the students to acquire and demonstrate the capability to use some other software applications, and to compute more advanced properties. The students are also trained to consult on-line documentation and compare their results with those available on the Web or in publications.

B. Background for the lab

During the lectures on April 16, 21, 23 and 24, the students will receive theoretical explanations, as well as practical guidance for the usage of ABINIT. This software application has a wealth of capabilities for the computation of properties of materials, and is free. Still, the underlying theory and the practical usage does not differ much from the ones of other software applications (VASP, Quantum Espresso, FHI-AIMS, SIESTA, etc). The on-line documentation is exhaustive, and includes many online tutorials. As such, it constitutes a good alternative to VASP, and allows the student to get exposed to alternative implementation, and acquire the capability to learn by her/him self to use such software applications. The student will see lots of similarities and some differences.

(The on-line availability proves to be also a convenient choice in the context of the COVID-19 pandemy)

Among the advanced topics that will be covered, the following three topics are the most noticeable in the context of the lab:

(1) The capability to compute accurate band gaps, thanks to the GW approach. This is at variance with the prediction obtained from straight application of Density Functional Theory (DFT).

(2) The capability to obtain phonon frequencies, and even phonon band structures.

(3) The capability to obtain optical spectra of solids, in the independent particle approximation (or random phase approximation- RPA).

Not all topics covered in the four above-mentioned lectures are covered by the lab. These three topics are simply sufficiently well-defined, and reasonably advanced without being too complex.

Some precomputed reference data are available on the Web : the materials project (https://materialsproject.org/), referred to as MP below, provides DFT electronic band structure (VASP, with advertised erroneous gap) as well as phonon band structures (ABINIT, in the PBEsol approximation). GW corrected data for 78 materials are available in Phys. Rev. B 96, 155207 (2017) - see the Supplementary material. These will be used as references.

Also, reference ABINIT input variables rprim, xred, natom, etc can be extracted from the "Abinit DDB" file provided in the "phonon dispersion" section of the MP, e.g. for MgO, https://materialsproject.org/materials/mp-1265/#phonon-dispersion for more than 1500 materials, although this covers only materials with a gap.

C. Description of the lab

Each student will select a material, and for this material, a specific crystalline phase such that the primitive unit cell has less than 6 atoms (preferably less than 4 atoms). Preferentially, the material must be chosen among those for which the phonon band structure is available on the MP (so that the above-mentioned rprim and xred ABINIT input variables are available), and this material should be connected to her/his center of interest, broadly speaking.

Also, a property among the three given above should be selected by the student. If the chosen property is the band gap, then the phase must have a gap (=be semi-conducting) in the electronic structure shown on the Materials Project (not simply for the above-mentioned convenience reasons).

The student will have to:

(i) compute the relaxed lattice parameters and relaxed internal atomic positions of this crystalline phase, in the LDA or in the GGA (not PBEsol);

(ii) compute one of the properties (1)-(3);

(iii) bring evidence that the cut-off energy, the wavevector sampling, and possibly other relevant convergence parameter(s) are sufficient to provide these lattice parameters, atomic positions, and other target property with a meaningful numerical accuracy (e.g. lattice parameters should be converged within 0.2% of the fully converged result).

(iv) provide comparisons with the data available on the MP (available from VASP within PBE + PAW, and from ABINIT within PBEsol).

(v) optionally, the student can bring additional comparison with published results in the literature.

(vi) gather the results and above-mentioned evidence and comparisons in a report.

D. Web-based tutorial

Numerous ABINIT tutorials are available on the Web (https://docs.abinit.org/tutorial). The students is supposed to follow some of them at her/his own pace.

Familiarization with the basic working knowledge of ABINIT will be gained with the basic tutorials 1 to 3 (possibly 4 for metals), https://docs.abinit.org/tutorial/base1 to base4. While a student without knowledge of other first-principles software application is expected to spend 6-8 hours on these tutorials (verified), the knowledge gained in the Basic Material Modelling lecture with the use of VASP will allow getting familiarized with ABINIT in less than one half-day, perhaps as few as two hours, depending on the skills of the student.

Then, depending on the chosen property, additional tutorials will have to be followed by the student :

(1) For the accurate band gap computation ; https://docs.abinit.org/tutorial/gw1 .

(2) For the phonon band structure computation : https://docs.abinit.org/tutorial/rf1 and https://docs.abinit.org/tutorial/rf2 .

(3) For the optical properties : https://docs.abinit.org/tutorial/rf1 and https://docs.abinit.org/tutorial/optic

Other resources for the lab include :

- The access to the Oleg computer:

1) To access online to “Oleg” we suggest to use “Putty” (https://www.putty.org/) and to upload and download files we suggest “Filezilla” (https://filezilla-project.org/download.php?platform=win64). Login and passwords will be given the day of the introduction to the lab (16 of April).

2) When you will enter into “Oleg” for the first time you will have to create your own folder that it will be called “d_name.surname” and inside the folder you will copy the script file “job-abinit.sh” that you will use to run the ABINIT calculations and the script “job-fh-aims.sh” to run FH-AIMS calculations. Inside the scripts **you have not to modify the number of nodes and the number of cores for any reason**.

All users have to call the job with their name and surname thanks to the script — #SBATCH -J "name.surname".

3) Inside of folder “d_name_surname” create a folder for each job to allow the TA and professors to help you in case you need assistance. All jobs not correctly called and files not in the personal folder but in a wrong place will be immediately deleted without notice. Respect yourself and the others.

4) Batch commands :

sbatch job-abinit.sh	run your abinit job (last line of job-abinit.sh can be edited to meet your needs)
sqx	see whether your job is running/waiting

(NOTE. The initial version of job-abinit.sh has to be corrected : in the last line, replace "mpirun abinit" by "mpirun -n 1 abinit" to run in sequential, this allows error messages by default. It has been upgraded in the abinit-tests directory.).

- The pseudo-dojo, http://www.pseudo-dojo.org/, from which the ABINIT pseudopotentials can be obtained ;

- The on-line documentation of ABINIT, including the topics https://docs.abinit.org/topics/features, the user guides https://docs.abinit.org/, the input variable description https://docs.abinit.org/variables .

- The open-source Abipy library for analyzing the results from ABINIT, https://github.com/abinit/abipy, see also the gallery of plotting scripts http://abinit.github.io/abipy/gallery .

E. Planning and deadlines

Practical hands-on with direct on-line support (on demand) from the teaching assistant and teacher (XG) will be organized :

- on Thursday 16 April, 11:00-12:00;
- on Tuesday 21 April, 11:00-12:00;
- on Thursday 23 April, 11:00-12:00;
- on Friday 24 April, 11:00-12:00;

The teaching assistant will also give additional availability periods for on-line help, and the teacher (XG) will arrange additional on-line meetings if needed.

On Friday 17 April 9:00, the student sends to the teaching assistant the material project ID of the phase chosen, and the property he/she will study (band gap, phonon frequencies or optical spectrum, among the (1)-(3) above). In case of foreseen problem with this choice, the student will be contacted, and will have the opportunity to switch material or property.

On Friday 24 April 18:00, the student sends to the teaching assistant a brief report with the computed relaxed lattice parameters and relaxed internal atomic positions of this crystalline phase, in the LDA or in the GGA, and accompanying evidence of numerical accuracy, see section C, point (i) completed partly with (iii) and (iv). If the computation has not been successful, the student should comment about the situation. This brief report has the goal to identify as early as possible whether there is a problem with the lab. In case of problem the student will be personally contacted. If there is no problem, some minor remarks/advices might be issued by the teaching team. This brief report will not be rated. Still, not delivering it on time or sending a report that indicates a clear lack of involvement would influence negatively the final rating of the lab.

On Thursday 14 May 23:59, or before, the student uploads on canvas the full report on the lab.