Lecture "Advanced Material Modeling"
Skolkovo Institute of Science and Technology
Description of the Lab #1

A. Objectives

In the "Basic Materials modeling" lecture, the students have been initiated to the usage of some modeling software applications, for molecules and for solids. In particular, as concern the modeling of materials, they have learned how to use specifically VASP for the computation of basic properties of crystalline solids, namely total energy and lattice parameters. VASP is one of the most used software applications 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 for the study of crystalline materials, to consult on-line documentation and compare their results with those available on the Web or in publications. This is the goal of lab #1. Possibly, afterwards, this will allow the students to study more advanced properties, which might be the topics of their specific project for the lecture.

B. Background and resources for the lab

During the lectures on April 2, 6, 9 and 13, the students will receive theoretical explanations, practical guidance for the basic usage of ABINIT, as well as theoretical lectures for mor advanced usage. ABINIT 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 an 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)

Computational resources:

Each student will be allowed to have access to the Skoltech virtual machine where he/she will be able to perform all necessary calculations for the lab. Detailed information how to have access will be found at the http://zhugayevych.me/edu/CC/Software.htm.

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 (from VASP, in the GGA-PBE approximation, with advertised erroneous DFT gap) as well as phonon band structures (from ABINIT, in the GGA-PBEsol approximation).

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.

Other important resources:

- The pseudo-dojo, http://www.pseudo-dojo.org/, from which the ABINIT pseudopotentials can be obtained (take only type PAW JTH v1.0, XC PBE, Accuracy Standard, Format psp8);
- The pseudopotentials for band structure calculations performed with TB09 (metaGGA DFT functional) must be taken from website

http://nninc.cnf.cornell.edu/dd_search.php?frmxcprox=&frmxctype=&frmspclass=HGH.

- 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.

C. Description of the lab

The student has to:

(i) Select a material, and for this material, select a specific crystalline insulating phase such that the primitive unit cell has less than 4 atoms. 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, see the "Abinit DDB" file in the phonon band structure section of the MP), and this material should be ideally connected to her/his center of interest, broadly speaking.

(ii) Start from the ABINIT rprim and xred available from the MP, and compute the total energy (with the GGA-PBE exchange-correlation functional) for a large set of values of cut off energy, on one hand, and k point sampling, on the other hand. Determine the needed cut-off energy and k point sampling to obtain a numerical accuracy better than 0.5 mHa per atom for this total energy

(iii) Compute the relaxed lattice parameters and possibly the relaxed internal atomic positions of this crystalline phase, in the GGA-PBE (not PBEsol), using these cut-off energy and k-point sampling.

(iv) Reexamine the cut-off energy and the wavevector sampling in order to provide these lattice parameters, atomic positions, and other target properties with a meaningful numerical accuracy (e.g. lattice parameters should be converged within 0.2% of the fully converged result).

(v) Produce an electronic band structure with PBE using PAW pseudo potentials and with meta-GGA TB09.

(vi) Provide comparison with the data available on the MP (available from VASP within GGA-PBE + PAW, and from ABINIT within PBEsol), e.g. cut and paste the band structure from the MP, and report in a table the acell and xred from ABINIT within PBEsol.

(vii) Optionally, the student can bring additional comparison with published results in the literature.

(viii) 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 https://docs.abinit.org/tutorial/base1 to base3. While a student without knowledge of other first-principles software application is expected to spend 6 hours on these tutorials (verified), the knowledge gained in the Basic Material Modelling lecture with the use of VASP might allow getting familiarized with ABINIT in about 4 hours, depending on the skills of the student.

E. Planning and deadlines

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

- on Friday 2 April, 11:00-12:00;
- on Tuesday 6 April, 11:00-12:00;
- on Friday 9 April, 11:00-12:00;
- on Tuesday 13 April, 11:00-12:00;

There will also be additional availability periods for on-line help if needed.

On Tuesday 6 April 9:00, the students send to Dr. Christian Tantardini (Christian.Tantardini@skoltech.ru) the material project ID of the phase chosen.

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 16 April 18:00, the students send to Dr. Christian Tantardini a first version of the report. It should contain **all results**: computed relaxed lattice parameters and relaxed internal atomic positions of this crystalline phase, in the GGA, band structure performed with PBE (GGA) and TB09 (meta-GGA), accompanying evidence of numerical accuracy, comparison. 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 22 April 18:00, or before, the student uploads on canvas the full report on the lab. After the submission no other chances to upload new versions with corrections.

F. Follow-up : projects for the lecture.

In due time, the students will choose a project for the lecture. As a follow-up of the lab#1, three sets of projects might be chosen, allowing application of the most advanced parts of the theoretical lectures of 6, 9 and 13 April :

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

(2) Computing phonon frequencies for the chosen material, and even phonon band structures.

(3) Computing optical spectra for the chosen material, in the independent particle approximation (or random phase approximation- RPA).

Depending on the chosen property, the following 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

As references for the comparison of obtained results, the above-mentioned phonon band structure from the MP are available. Also, GW corrected data for 78 materials are available in Phys. Rev. B 96, 155207 (2017) - see the Supplementary material. References for the optical properties are not available on the Web, but should be searched in the literature.