A Step-by-Step Guide for *ab initio* Calculation of the Hole Mobility of Si using Quantum ESPRESSO and aMoBT on nanoHub.org

Alireza Faghaninia

CAML Lab, Washington University in St. Louis

Remarks

- Hole mobility of Si is just one example that was chosen for availability and simplicity of Quantum ESPRESSO (QE) calculation of this material on nanoHub
- Similar steps can be taken for calculating electronic properties of other semiconductors
- Both VASP and QE are compatible with aMoBT: ab initio model for calculating the mobility in Boltzmann Transport framework
- Steps:
  1. ab initio calculations
  2. aMoBT calculations

aMoBT

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Ab initio electronic transport model with explicit solution to the linearized Boltzmann transport equation

Alireza Faghaninia
Department of Energy, Environmental, and Chemical Engineering, Washington University, St. Louis, Missouri 63130, USA

Joel W. Ager III
Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

Cynthia S. Lo*
Department of Energy, Environmental, and Chemical Engineering, Washington University, St. Louis, Missouri 63130, USA
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Accurate models of carrier transport are essential for describing the electronic properties of semiconductor materials. To the best of our knowledge, the current models following the framework of the Boltzmann transport equation (BTE) either rely heavily on experimental data (i.e., semiempirical), or utilize simplifying assumptions, such as the constant relaxation time approximation (BTE-cRTA). While these models offer valuable physical insights and accurate calculations of transport properties in some cases, they often lack sufficient accuracy—particularly in capturing the correct trends with temperature and carrier concentration. We present here a transport model for calculating low-field electrical drift mobility and Seebeck coefficient of *n*-type semiconductors, by explicitly considering relevant physical phenomena (i.e., elastic and inelastic scattering mechanisms). We first rewrite expressions for the rates of elastic scattering mechanisms, in terms of *ab initio* properties, such as the band structure, density of states, and polar optical phonon frequency. We then solve the linear BTE to obtain the perturbation to the electron distribution—resulting from the dominant scattering mechanisms—and use this to calculate the overall mobility and Seebeck coefficient. Therefore, we have developed an *ab initio* model for calculating mobility and Seebeck coefficient using the Boltzmann transport (aMoBT) equation. Using aMoBT, we accurately calculate electrical transport properties of the compound *n*-type semiconductors, GaAs and InN, over various ranges of temperature and carrier concentration. aMoBT is fully predictive and provides high accuracy when compared to experimental measurements on both GaAs and InN, and vastly outperforms both semiempirical models and the BTE-cRTA. Therefore, we assert that this approach represents a first step towards a fully *ab initio* carrier transport model that is valid in all compound semiconductors.

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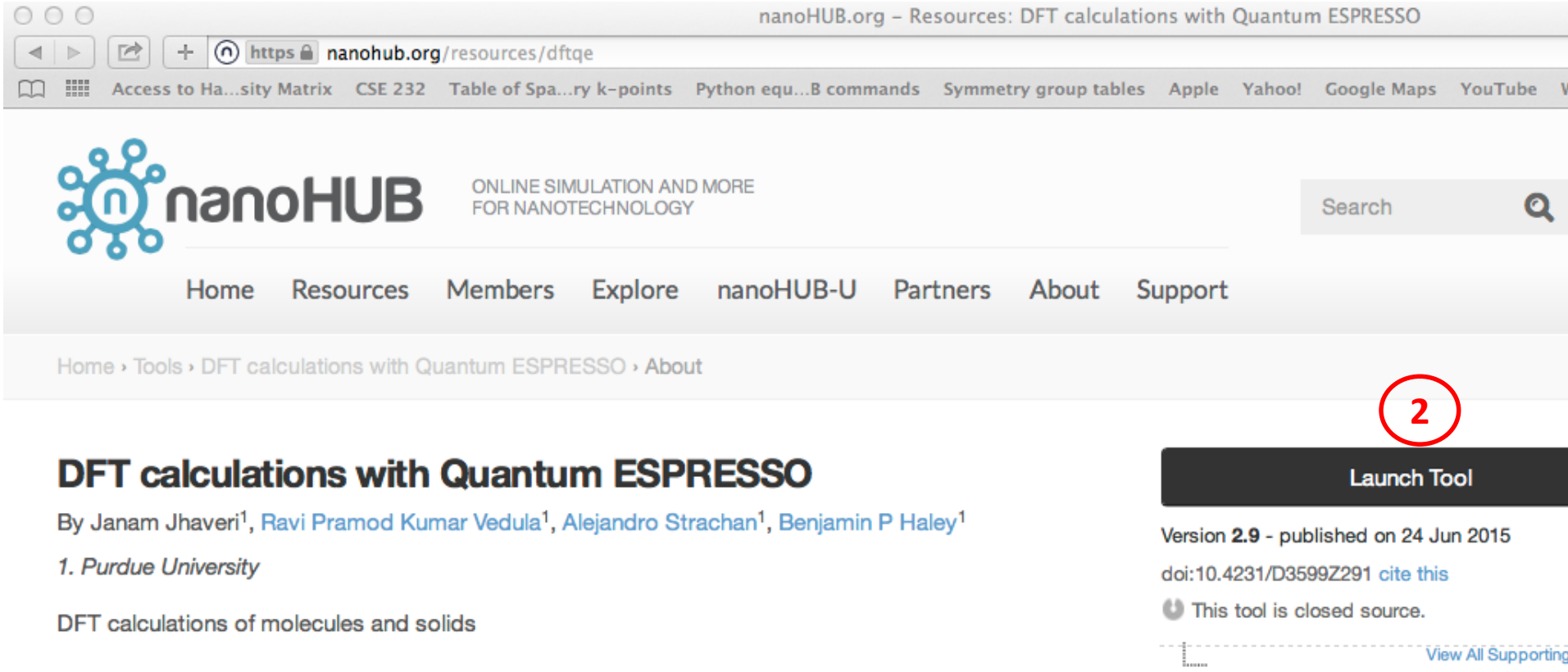
Section 1:
Generating the Quantum ESPRESSO output on nanoHub.org

You can skip to Section 2 if you use VASP or if you use Quantum ESPRESSO in Unix.

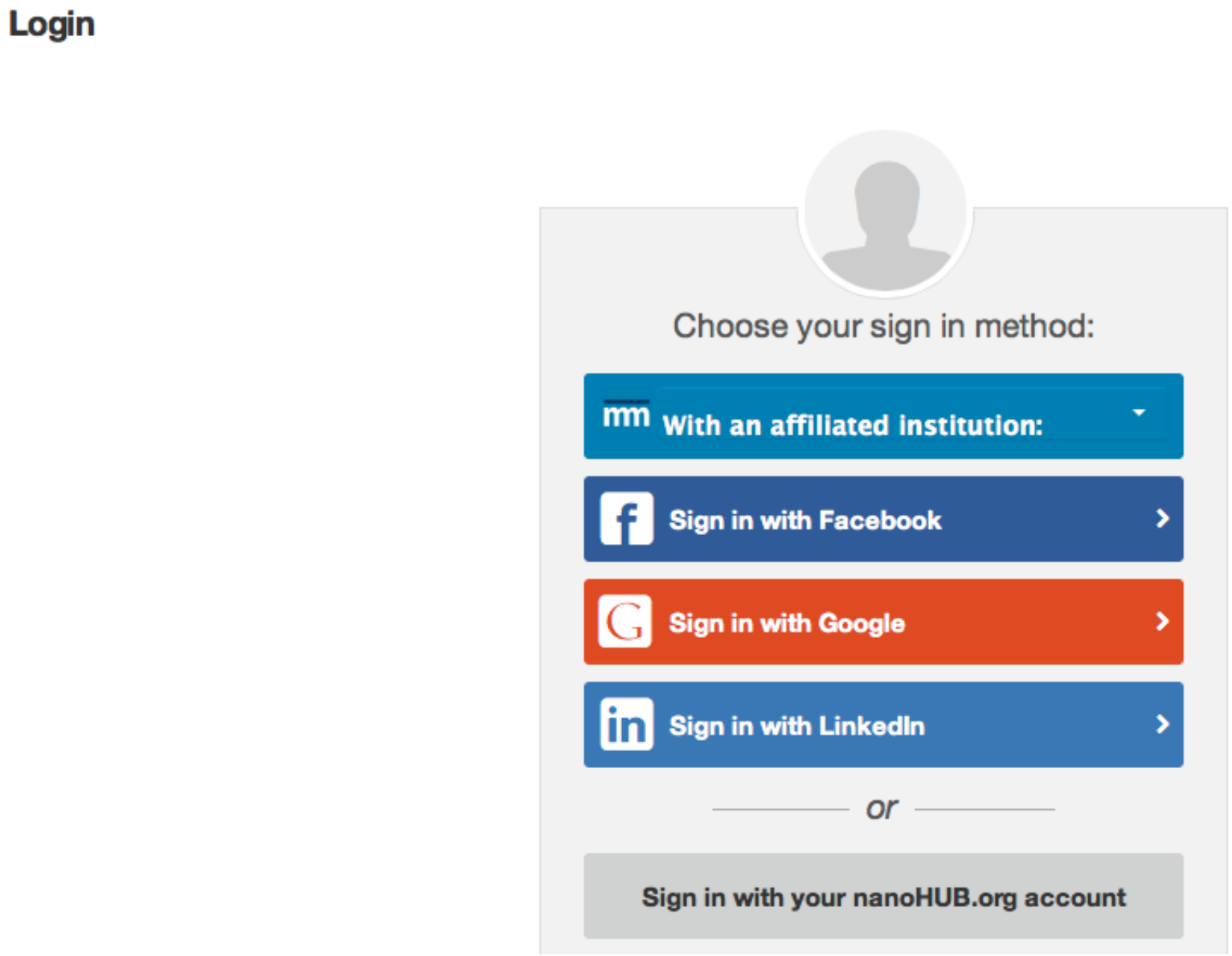
* If you use QE in Unix, start from slide 12.

1) ab initio calc.: QE on nanoHub for simplicity

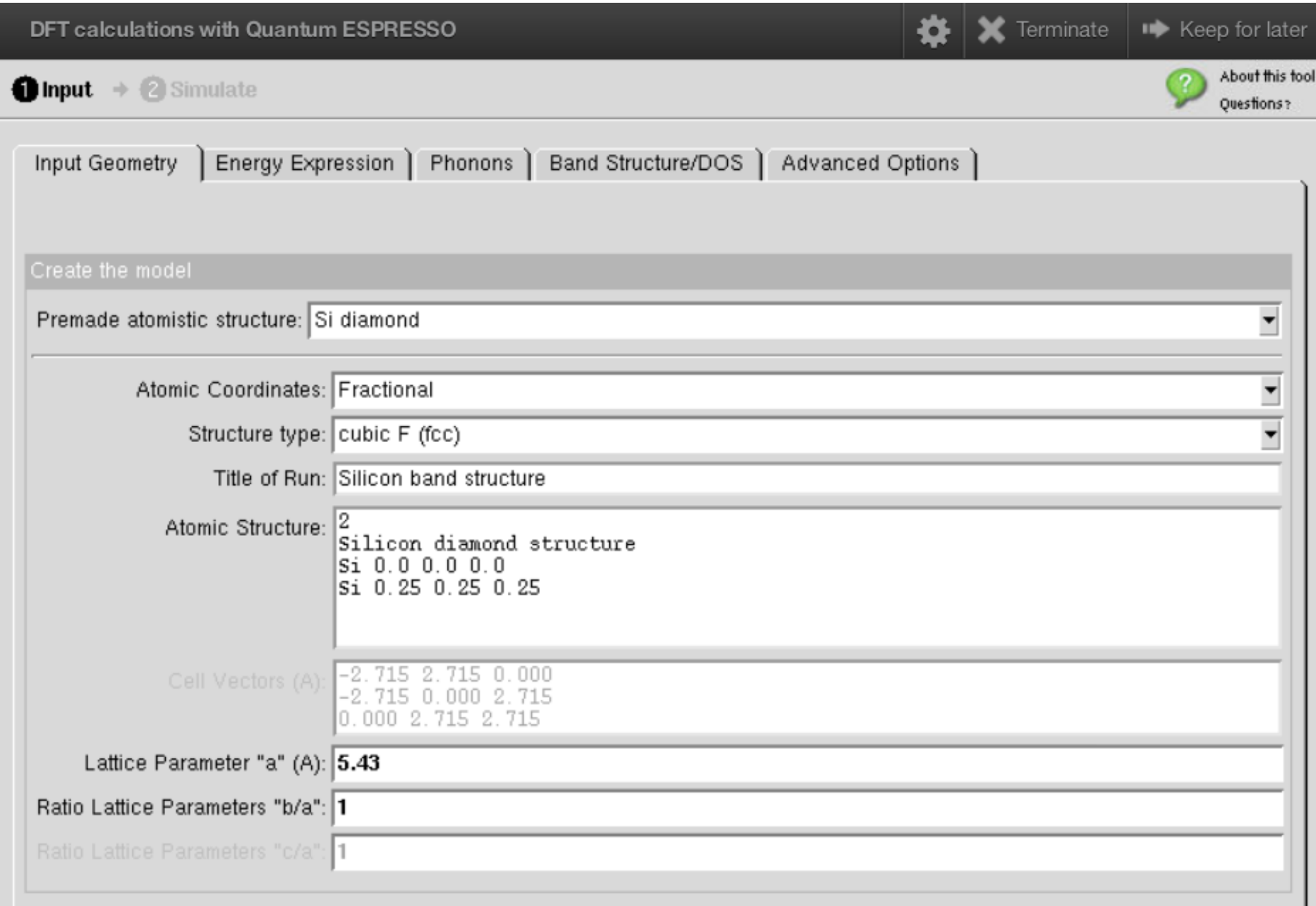
1. Open https://nanohub.org/resources/dftqe
2. Select Launch Tool



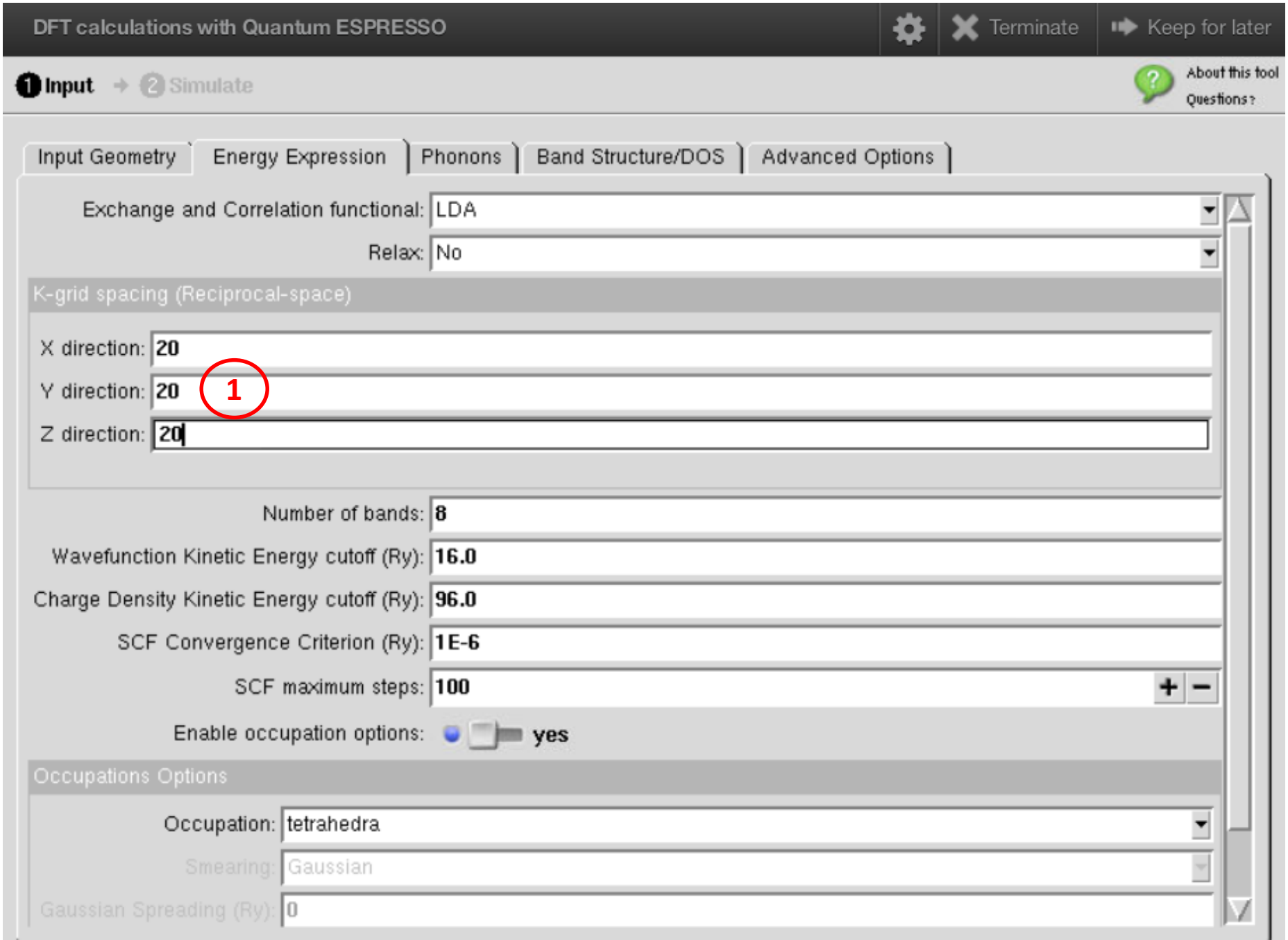
- You need to sign-in using one of the following methods or simply signup in the website free of charge.



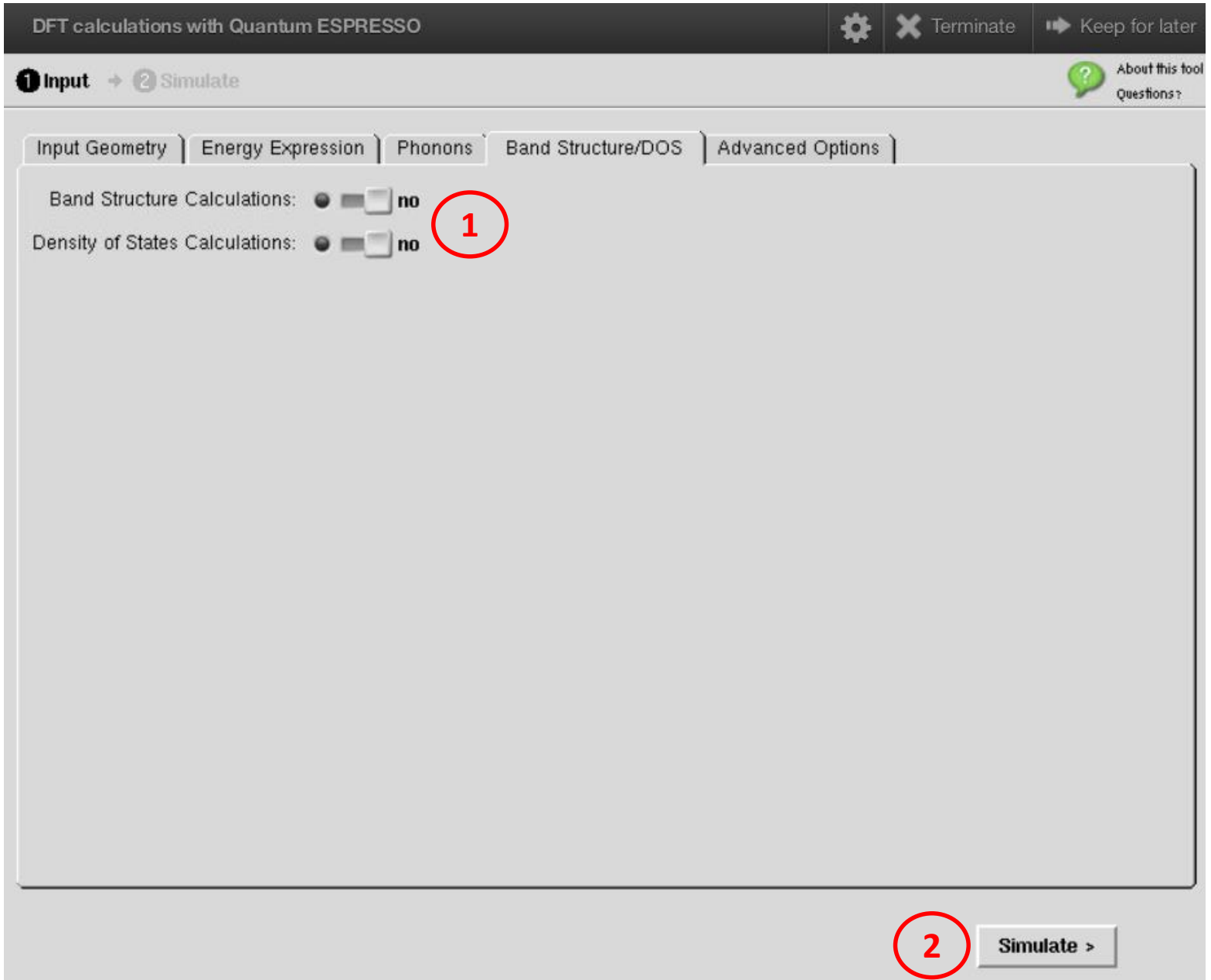
- Leave the first tab as default. It should look like the one below



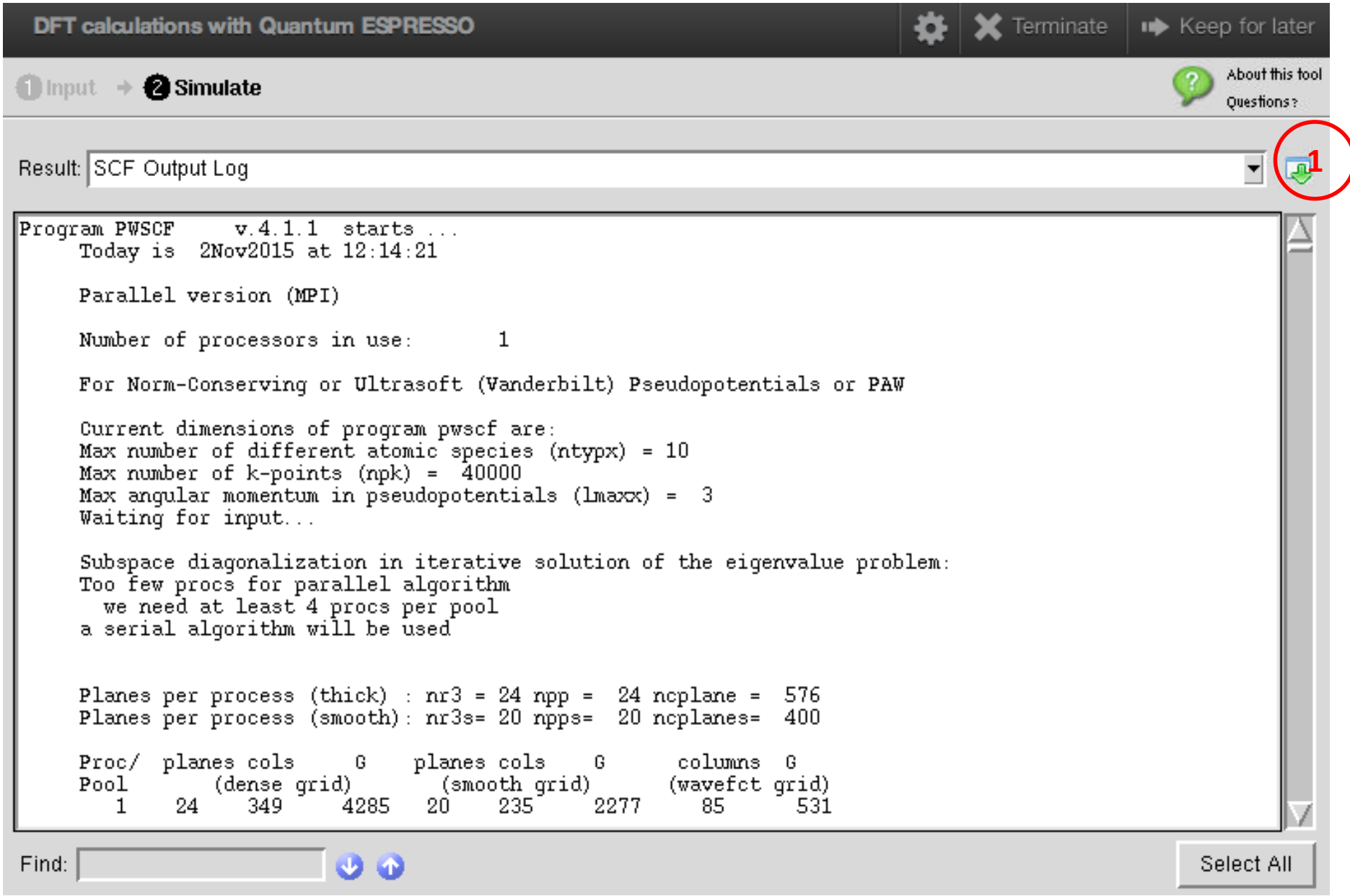
1. Change the number of kpoints to 20 in each direction (see below)



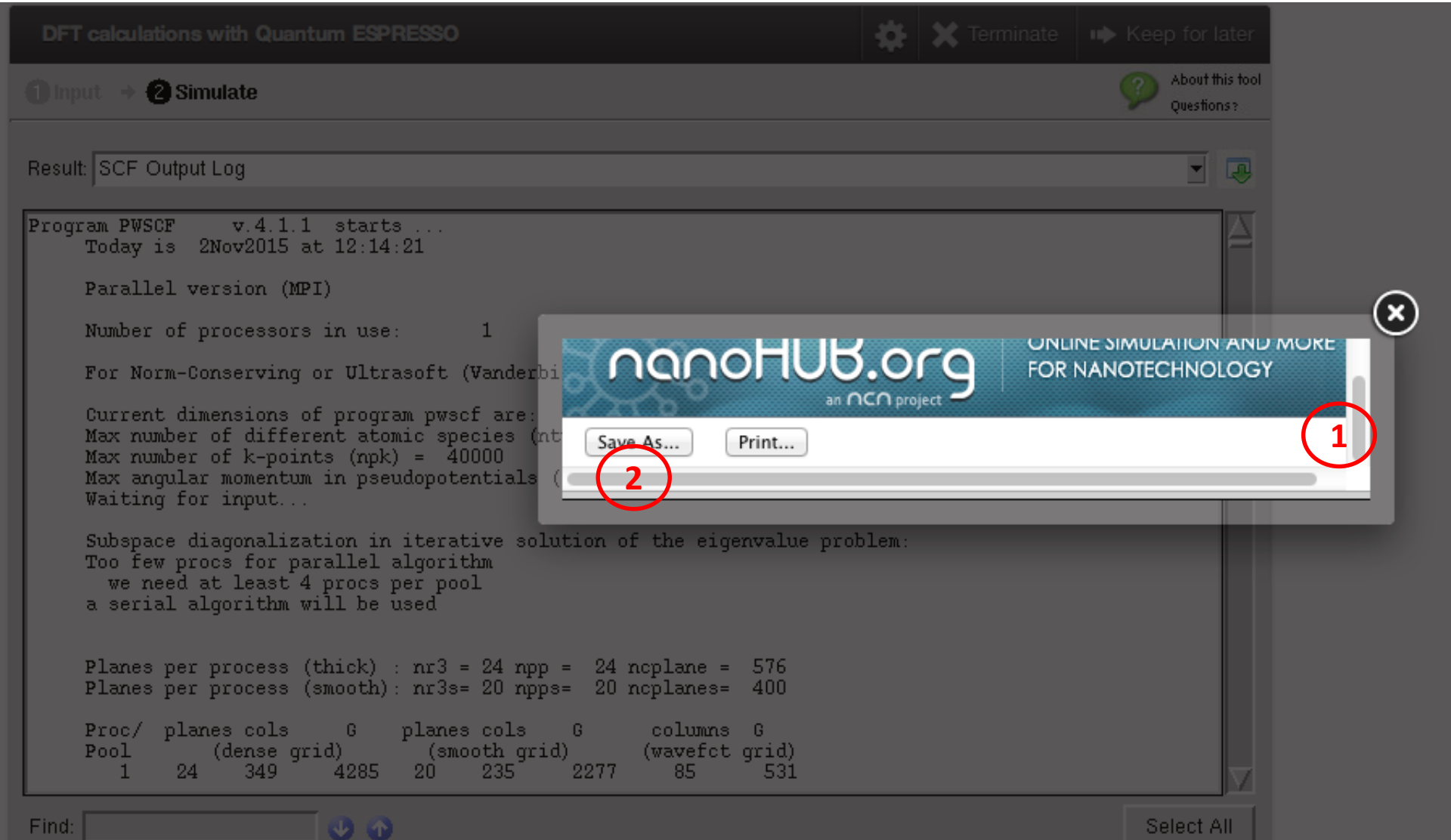
1. Choose not to calculate the band structure or density of states (DOS)
2. Simulate



1. Select the download button to download the output



1. In the popped-up window, you may need to scroll down to see the “Save As …” button.
2. Click on the “Save As …” button and choose where you want to download the output file.



1. Download “QE-to-VASP.py” python code from here:
https://nanohub.org/resources/amobt/supportingdocs
2. Once “QE-to-VASP.py” and your QE output file (which we call “SCFOutputLog.txt” here) in the same folder run the python code as follows:

    python QE-to-VASP.py -f SCFOutputLog.txt

    or basically:

    python QE-to-VASP.py -f your_QE_output_file

This should generate the EIGENVAL and OUTCAR files which contain information regarding the lattice dimensions and itds volume. These two files are minimum requirements for aMoBT for calculating the mobility and Seebeck coefficient (next section).

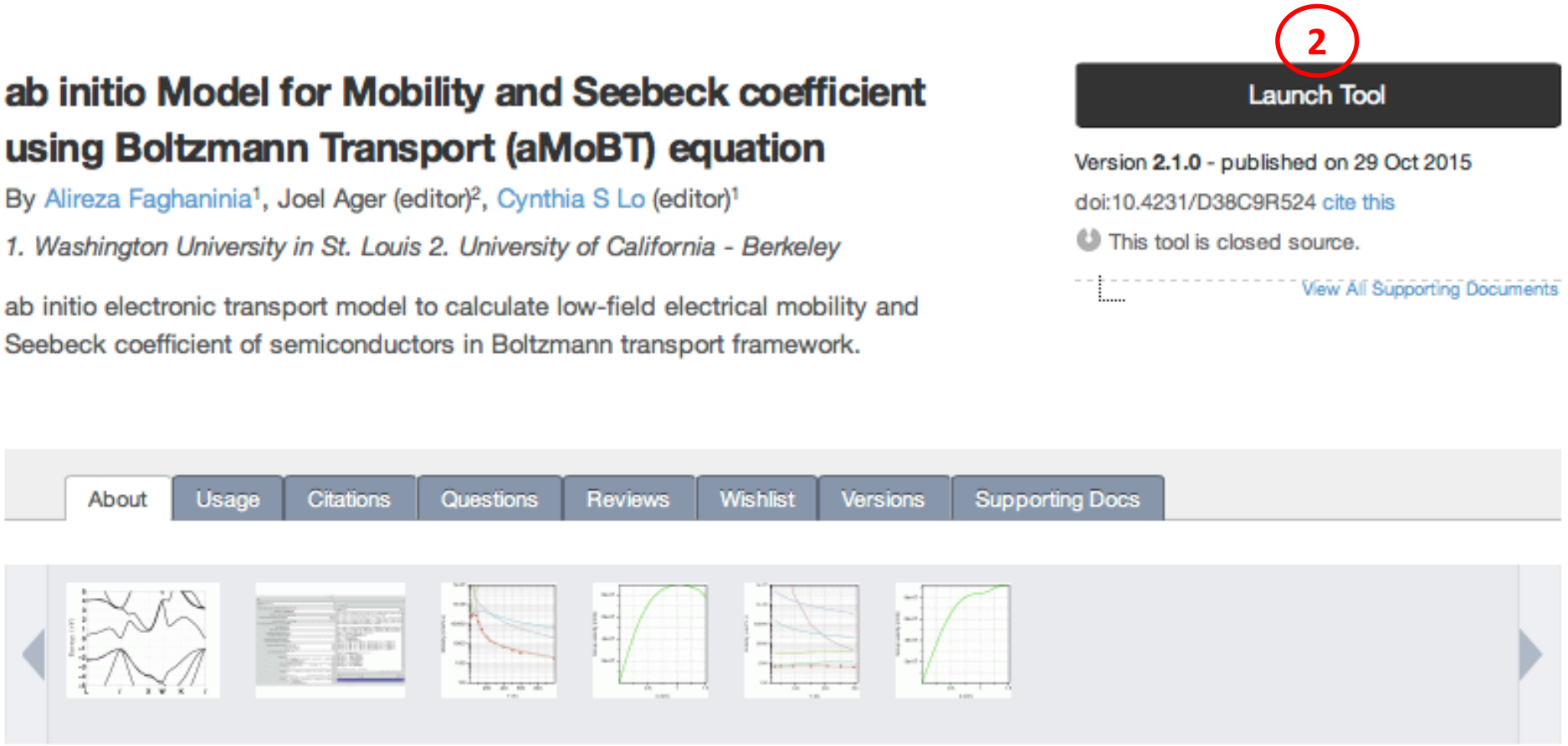
3. If you don’t have python, you can download the resulting EIGENVAL and OUTCAR from the following links to continue this example:
https://www.dropbox.com/s/8v0l4a3xecmhb1b/EIGENVAL?dl=0
https://www.dropbox.com/s/ka025rbtf1r3uvj/OUTCAR?dl=0

Section 2:
Calculating the mobility and Seebeck coefficient using aMoBT

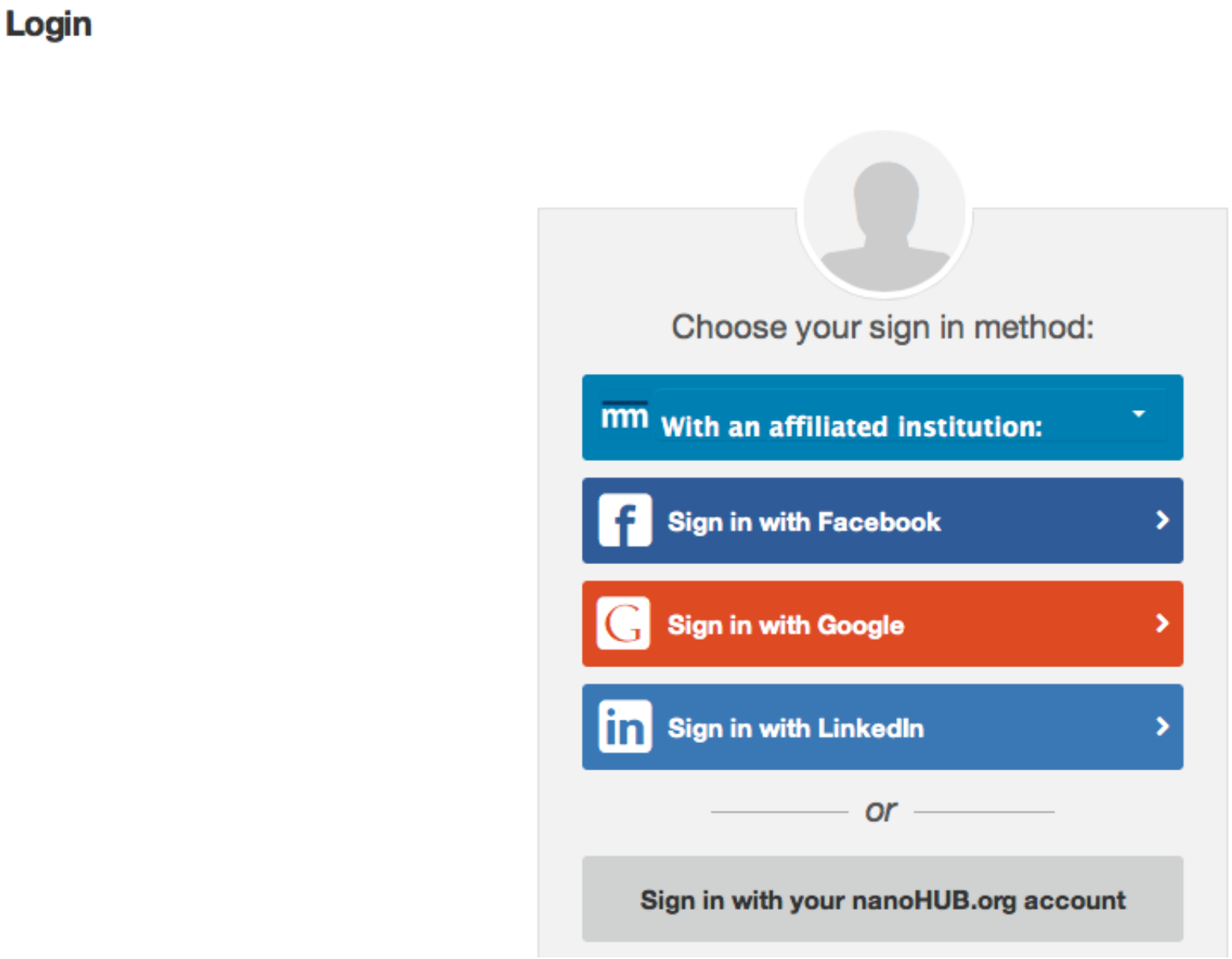
It is assumed in this section that you have the EIGENVAL and OUTCAR files ready for upload.

2) aMoBT calculations

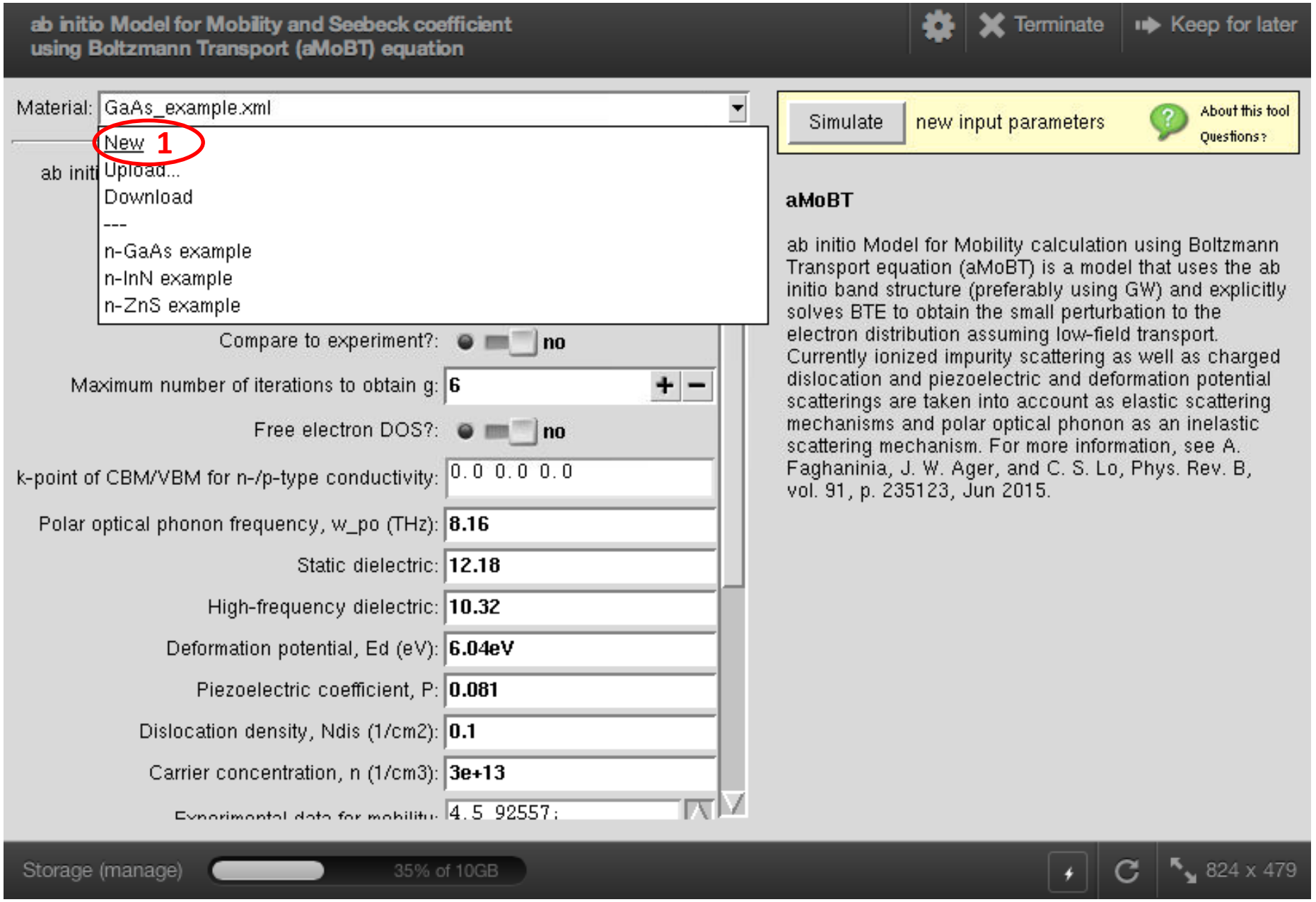
1. Open https://nanohub.org/tools/amobt
2. Select Launch Tool



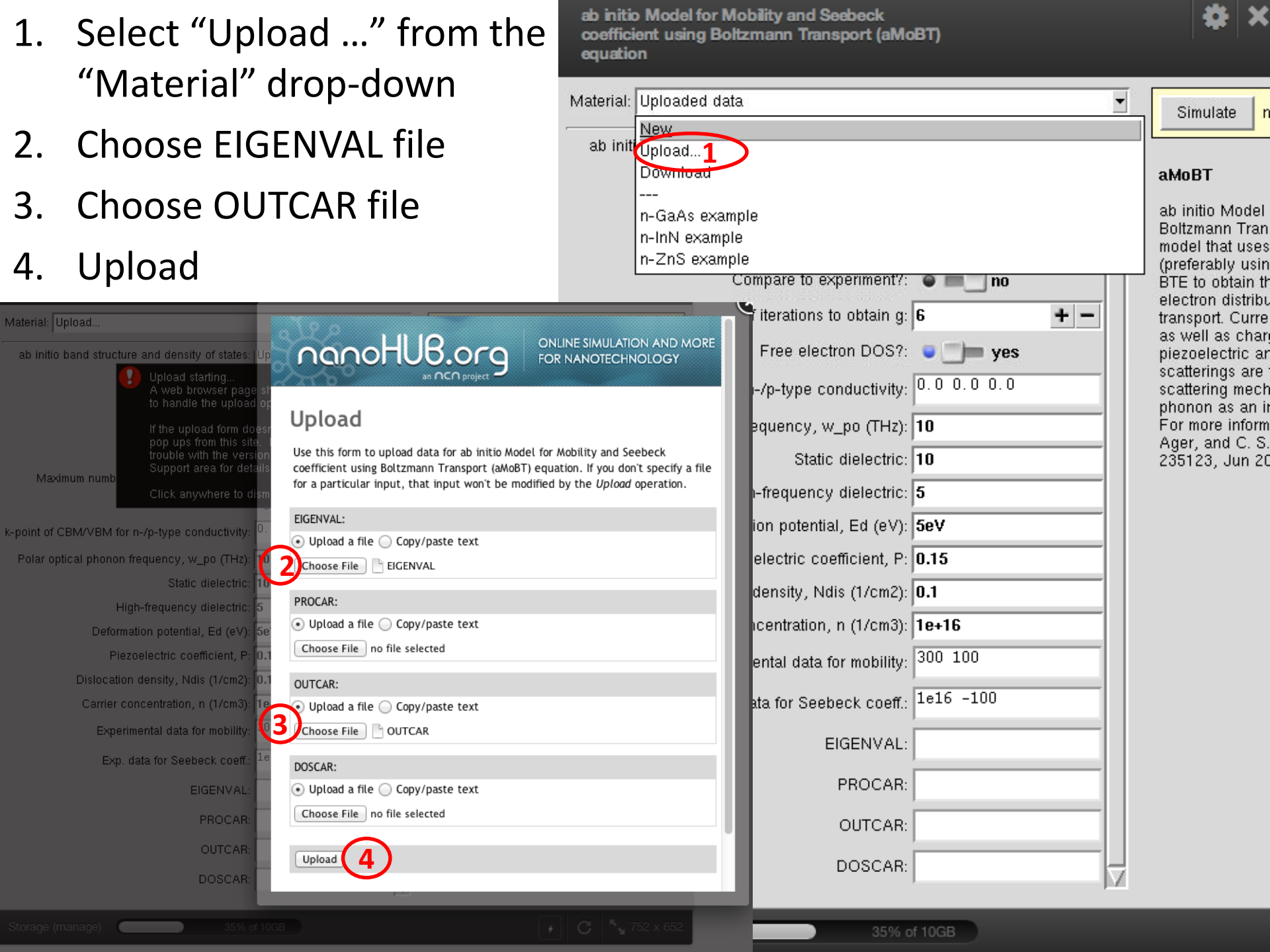
1. You need to sign-in using one of the following methods or simply signup in the website free of charge.



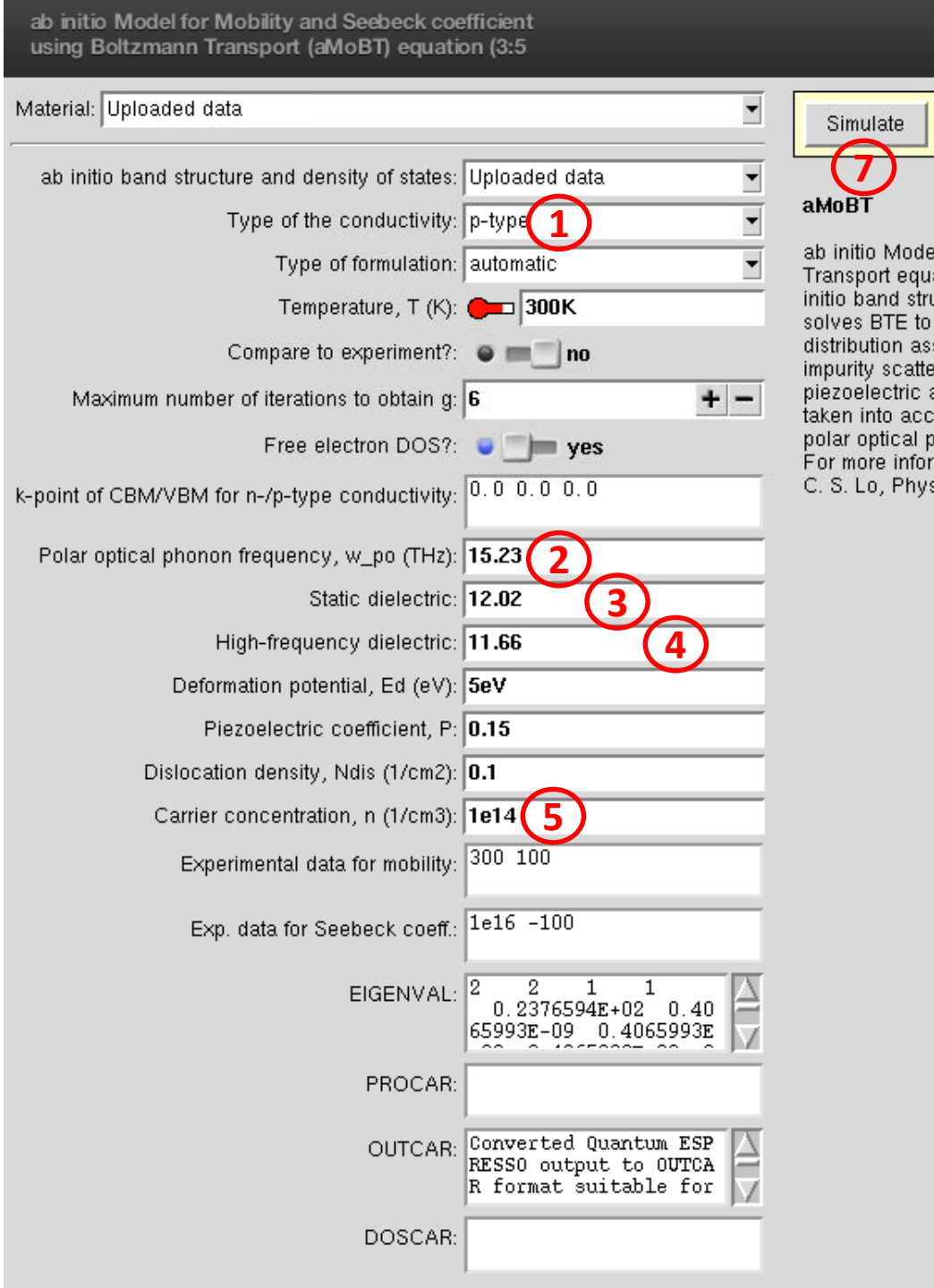
1. From the “Material” drop-down menu, select “New”



1. Select “Upload …” from the “Material” drop-down
2. Choose EIGENVAL file
3. Choose OUTCAR file
4. Upload

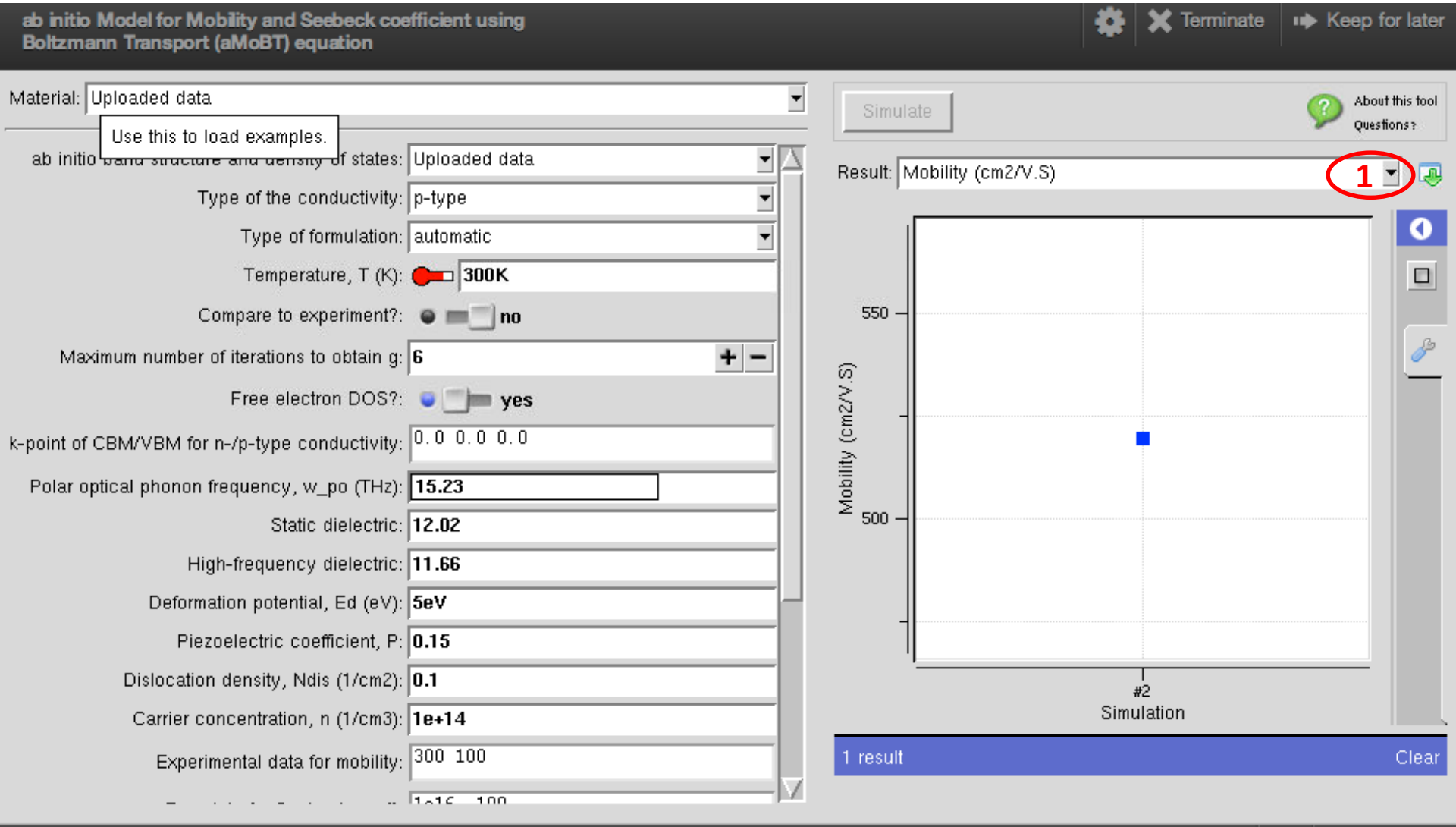


1. Select “Type of the conductivity” to be : “p-type”
2. Optical phonon frequency at Γ : 15.23 THz
   - Calculated via DFPT(VASP)+Phonopy
3. Static dielectric: 12.02
   - Calculated via DFPT(VASP)
4. High frequency dielectric: 11.66 (=12.02x(15/15.23)^2)
   - Calculated via Lyddane–Sachs–Teller relation: $(\omega_{LO}/\omega_{TO})^2=\varepsilon_s/\varepsilon_\infty$
5. Carrier Concenteration: 1e14
6. Leave the rest to default
7. Simulate



- The calculation should finish in about 53 seconds
- The hole mobility of Si is 450 $cm^2/V.s$ at 300K

1. Use the drop-down menu to see other outputs (e.g. group velocity)



- You can use a similar procedure to calculate the mobility and Seebeck coefficient of other semiconductors.
- The output depends on the accuracy of the calculated band structure and other properties such as phonon frequencies and dielectric constants.
- Questions? please see the manual
  https://nanohub.org/resources/amobt/supportingdocs
  or contact alireza@wustl.edu