NOTE:

This software requires output files from Gaussian16 quantum chemistry package. The following instructions provide an overview of how to perform the primary required calculations in Gaussian16 and the transmission calculations through the MATLAB GUI.

- Create directory for optimized geometry.
- Build molecule and set up calculation details. This step should be the optimization step. **DO NOT** include keywords to generate Fock and overlap matrices yet. If you do, the output file will be huge even for small calculations.
- Create new directory for transmission calculations
- Make a copy of the .chk file from the optimization step and paste into the new directory.
- Open the output file of previous calculation in gaussview and open a new molecule window in gaussview by going to *File -> New Molecule Group*. Copy the geometry from the output window into the new molecule window. This can be done with Ctrl-C and Ctrl-V.
- Now we want to calculate the information necessary for the transmission step. In the "additional keywords" section of the Gaussian calculation setup window, include the following statements
    - gfprint
    - iop(5/33=3, 3/33=1)
    - guess=read

  each keyword should be separated by a space. The same level of theory (functional and basis set) should be used as in the optimization step. The first keyword tells prints out the information of the basis functions assigned to each atom which we use to construct the coupling matrices. The second keyword prints out the Fock and overlap matrices. The third keyword tells Gaussian to read the .chk file when for the orbital coefficients during the SCF procedure. Since these orbitals are already optimized it will greatly speed up the calculation.

- You will need to specify which .chk file to read from. This is done under the "Link 0" tab of the calculation setup. Under the line that reads checkpoint file, select "Specify…" under the drop down menu. Click the […] button to select the appropriate file from the folder manager. MAKE SURE you select the .chk file that you copied into the new directory.
- Save the file in the new directory and run the calculation.
- Next open the transmission software titled "Transport_Simulation_GUI_v3.mlapp"
- At the top of the screen, select the "Get Input File" button and select the output file of the calculation you just completed. NOTE: it make take a moment to read all the necessary information from the output file. Once the file is read in, the path and filename will be displayed on screen.
- Next input the parameters for transmission calculation on the right. The parameters worth noting here are the injection and extraction sites. These correspond to the terminal atoms that are directly coupled to the electrodes. They are listed in sequential order in the input file of the Gaussian simulation. Alternatively, you can open the input or output file in Gaussview to determine the atom numbers for the injection/extraction sites by hovering your mouse cursor over the desired atom and it's index will be listed at the bottom left corner of the screen.
- Input the remaining information you need for the calculation, namely, the energy range (min and max), the resolution (spacing), the coupling to the injection/extraction sites, the broadening, the

Fermi level, and the temperature. The bias and buttiker probe sites section currently do not affect the calculation.

- Press the simulate button and wait. When completed, a graph of the transmission plot will be displayed on screen along with several values of interest below it, namely, zero bias conductance, transmission at the fermi level, the Seekbeck coefficient, and the HOMO and LUMO energies.
- The data used to make the graph can be saved in a two-column format by providing a title in the bottom right corner of the GUI and clicking the “Save Transmission Data” button.