**COSMOSS user guide**

**Introduction & quick starting guide:**

COSMOSS stands for Coupled OScillator MOdel Spectrum Simulator.

Given a molecule structure, this Matlab code can generates different kinds of vibrational spectrum base on coupled oscillator model. COSMOSS can be used to simulate:

1. Fourier Transform Infared spectrum (FTIR)

2. Sum-Frequency Generation spectrum (SFG)

3. Two dimentional Infared spectrum (2DIR)

4. Two dimentional Sum-Frequency Generation spectrum (2DSFG)

The supported molecule structure including:

1. Two coupled oscillators

2. ideal Betasheet

Beside these default structure models, this code is design to be used for other molecules as well. You can build any molecule and simulate their spectra. Please check sub-function in MoleculeConstruction folder for more information

To use this code, simply download it into your Matlab path and excute COSMOSS.m.

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Note:

The GUI portion is created base on the “GUI Layout Toolbox”, wrote by David Sampson.

For this version (v1.2.5) you have to install the tool box to use COSMOSS.

Further information about GUI Layout Tool box can be found in:

<http://www.mathworks.com/matlabcentral/fileexchange/47982-gui-layout-toolbox>

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**Simulation work flow**

There are three major part of COSMOSS:

1. Main : Spectrum simulation (COSMOSS.m)
2. Model : Molecule construction (Model\_XXX.m)
3. Modes: Mode Visualization (Plot\_Mode.m)

The working flow start from initiating COSMOSS.m that bring up the Main GUI. Then select a molecule construction model, which will bring up a molecule construction GUI. Using the Model GUI to construct a molecule and check the structure by drawing it. At this point you can start to generate spectrum on the main GUI. If you need to visualize the transition dipoles or Raman tensor of the molecule, you can bring up the third GUI Plot\_Mode.m by clicking the Plot Mode button on Model GUI. Once the mode visualization GUI appear, you can visualize what the orientation of a selected Exciton(Local) mode is. You can also rotate the molecule structure by Model GUI and go back to mode visualization GUI to see how does the corresponding mode change.

**Notes**

**Coupling Models**

There are 4 coupling models in COSMOSS: TDC, NN\_Mix\_TDC\_betasheet, Cho\_PB, Cho\_APB. The TDC model stand for transition dipole coupling. This model works well on describing middle to long range coupling between modes. It is well known that TDC model over estimates the coupling size if the distance between modes are short (~<5). As a result, the second model: NN\_Mix\_TDC\_betasheet is provided to correct nearest neighbor coupling on TDC model. The NN\_Mix\_TDC model allow user to manually substitute the nearest neighbor coupling size in TDC model.

For betasheet simulation, Cho’s group published a coupling map base on quantum simulation1. This map is also included in COSMOSS for benchmark and comparison. The PB refers to parallel betasheet while the APB is the antiparallel one. This map is extracted from an ideal betasheet structure and thus can **only** be used in ideal betasheet model.

**Simulation of Isotope labeling**

The isotope labeling is assigned in Model GUI. To simulate isotope labeling, you can designate the labeled local mode frequency in “labeled Freq” and which mode is labeled in “Labeling Index”. Here’s an example for a 3 strands ideal betasheet with 6 residues per strand. If the isotope labeled sit on the fourth amino acid of each strand, then the “Labeling Index” will be: 4, 10, 16.

**Reference:**

(1) Hahn, S.; Kim, S.-S.; Lee, C.; Cho, M. Characteristic Two-Dimensional IR Spectroscopic Features of Antiparallel and Parallel Beta-Sheet Polypeptides: Simulation Studies. *J. Chem. Phys.* **2005**, *123*, 084905.