1. **Generate random Al distribution**

Requirement: Jupyter Notebook, Python

* 1. Copy the file “LTA\_my.cif” to the folder “C:\\LTA\\”
  2. Change the variable i (to determine the number of Al to be replaced by Si script) in the script “Generate random Al distribution.ipynb”.
  3. Run the script “Generate random Al distribution.ipynb” using Jupyter Notebook, pick the Al distribution with the closest Warren-Clwley parameter to the average.
  4. Override the atom distribution content in “LTA\_my.cif” with the Al distribution content picked.

1. **Equilibrium cation distribution using parallel tempering**

Requirement: RASPA

* 1. Copy the file “LTA\_my.cif” in 1.4 to the folder “Restart”
  2. Change the value of “CreateNumberOfMolecules” (to determine the number of Na and K in a unit cell) in the script “Restart\\ simulation.input”.
  3. Run the simulation using RASPA,

1. **Identify cation distribution**

Requirement: Mofagraphy

1. **Predict adsorption uptake using GCMC simulation**

Requirement: RASPA

* 1. Copy the file “LTA\_my.cif” in 1.4 to the folders “co2” and “n2”.
  2. Copy the file “Restart\\Restart\\System\_0\\ restart\_LTA\_my\_1.1.1\_303.000000\_0” to the folders “co2\\RestartInitial\\System\_0\\” and “n2\\RestartInitial\\System\_0\\”; change the name of the file in both folders to “restart\_LTA\_my\_1.1.1\_298.150000\_100000”.
  3. Run the simulations using RASPA,

1. **Obtain DSL model**

Requirement: Origin LAB

* 1. Collect the adsorption uptakes predicted in 4.3, and generate adsorption isotherms at 263.15K, 298.15K, 308.15K, and 323.15K.
  2. Fit these data points in a DSL model using Origin LAB.

1. **Process simulation and optimization**

Requirement: MATLAB

* 1. Override the DSL parameters the row 16 of the table “PSA\\Params.mat\\IsothermPar“ with your DSL model obtained in 5.2.
  2. Run the script “PSA\\run\_FullOptimization.sh” using MATLAB,