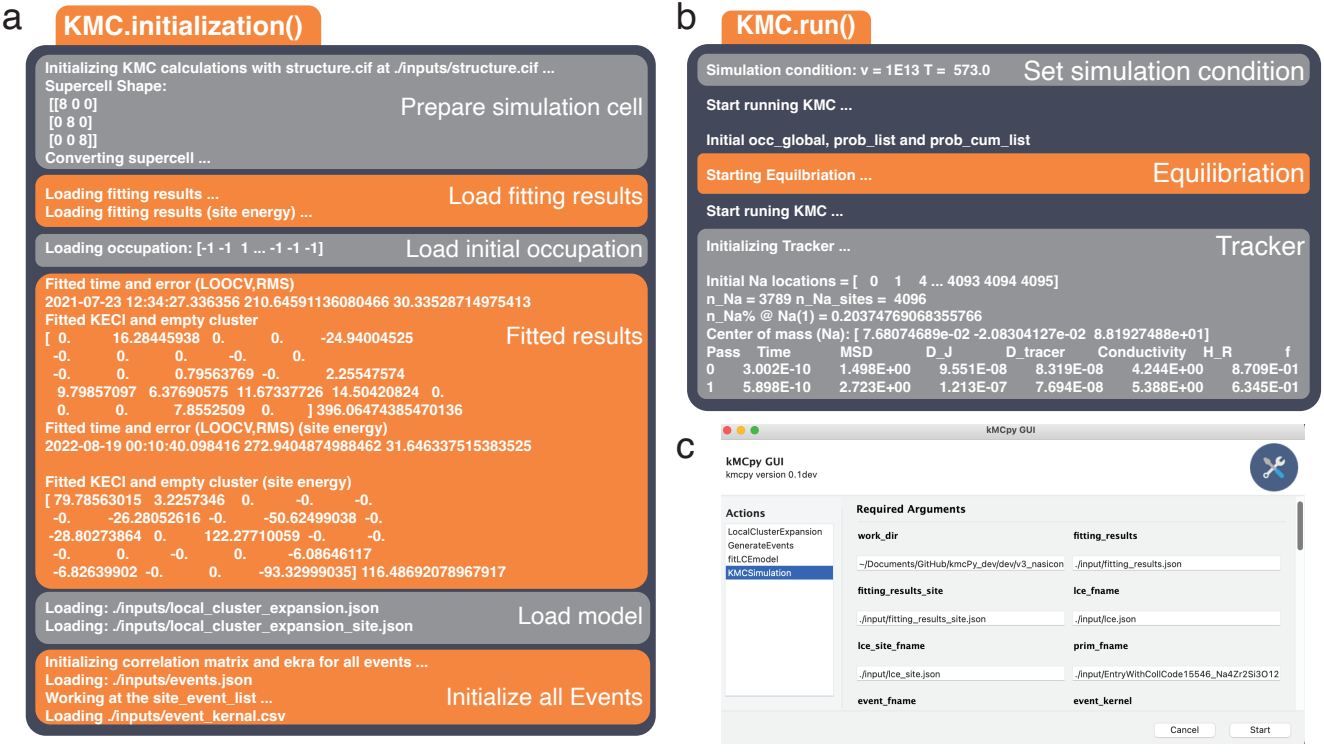
a
KMC.initialization()
Initializing KMC calculations with structure.cif at ./inputs/structure.cif ...
Supercell Shape:
[[8 0 0]
[0 8 0]
[0 0 8]]
Converting supercell ...
Prepare simulation cell
Loading fitting results ...
Loading fitting results (site energy) ...
Load fitting results
Loading occupation: [-1 -1 1 ... -1 -1 -1]
Load initial occupation
Fitted time and error (LOOCV,RMS)
2021-07-23 12:34:27.336356 210.64591136080466 30.33528714975413
Fitted KECI and empty cluster
[0. 16.28445938 0. 0. -24.94004525
-0. 0. 0. -0. 0.
-0. 0. 0.79563769 -0. 2.25547574
9.79857097 6.37690575 11.67337726 14.50420824 0.
0. 0. 7.8552509 0.] 396.06474385470136
Fitted time and error (LOOCV,RMS) (site energy)
2022-08-19 00:10:40.098416 272.9404874988462 31.646337515383525
Fitted KECI and empty cluster (site energy)
[79.78563015 3.2257346 0. -0. -0.
-0. -26.28052616 -0. -50.62499038 -0.
-28.80273864 0. 122.27710059 -0. -0.
-0. 0. -0. 0. -6.08646117
-6.82639902 -0. 0. -93.32999035] 116.48692078967917
Fitted results
Loading: ./inputs/local_cluster_expansion.json
Loading: ./inputs/local_cluster_expansion_site.json
Load model
Initializing correlation matrix and ekra for all events ...
Loading: ./inputs/events.json
Working at the site_event_list ...
Loading ./inputs/event_kernal.csv
Initialize all Events
b
KMC.run()
Simulation condition: v = 1E13 T = 573.0
Set simulation condition
Start running KMC ...
Initial occ_global, prob_list and prob_cum_list
Starting Equilbriation ...
Equilibriation
Start runing KMC ...
Initializing Tracker ...
Tracker
Initial Na locations = [0 1 4 ... 4093 4094 4095]
n_Na = 3789 n_Na_sites = 4096
n_Na% @ Na(1) = 0.20374769068355766
Center of mass (Na): [7.68074689e-02 -2.08304127e-02 8.81927488e+01]
Pass Time MSD D_J D_tracer Conductivity H_R f
0 3.002E-10 1.498E+00 9.551E-08 8.319E-08 4.244E+00 8.709E-01
1 5.898E-10 2.723E+00 1.213E-07 7.694E-08 5.388E+00 6.345E-01
c
kMCpy GUI
kMCpy GUI
kmcpy version 0.1dev
Actions
LocalClusterExpansion
GenerateEvents
fitLCEmodel
KMCSimulation
Required Arguments
work_dir
~/Documents/GitHub/kmcPy_dev/dev/v3_nasicon
fitting_results
./input/fitting_results.json
fitting_results_site
./input/fitting_results_site.json
lce_fname
./input/lce.json
lce_site_fname
./input/lce_site.json
prim_fname
./input/EntryWithCollCode15546_Na4Zr2Si3O12
event_fname
event_kernel
Cancel
Start