1 1D Model

Here we will demonstrate the basic idea of KMC and use it to model a microscopic random walk, then scale it to a diffusive process. The model is a one-dimensional line of sites with one particle hopping along the line at a time. The particle can either hop left or right at any given moment, if it gets to the end of the line then the particle is removed and a new particle is spawned at the centre of the line.

In the `kmc_constants` file you can alter the left and right hopping rates as well as the temperature. There are only two energies in the simulation, the energy of each site and the thermal energy $k_B T$, both expressed in terms of the reduced temperature. Recall that the rate of the left and right hops are:

$$\boldsymbol{R}_L = \boldsymbol{H}_L \min[1, \mathrm{e}^{-\frac{E_{x-1}-E_x}{k_B T}}] \tag{1}$$

$$\boldsymbol{R}_R = \boldsymbol{H}_R \min[1, \mathrm{e}^{-\frac{E_{x+1}-E_x}{k_B T}}] \tag{2}$$

where $\boldsymbol{H}$ denotes the base hopping rate in one direction and E_x is the energy of site x.

Remember to generate a waiting time from this we draw an exponentially distributed random number, a:

$$t_{\text{wait}} = \frac{a}{\boldsymbol{R}} \tag{3}$$

N.B. the waiting time is in units of 1 over the rate, in this model the rates define the time scale.

Play with some of the parameters of the model and see how changing the rates will affect the number of particles out per unit time.

If you look at the talk notes you can see how discrete hops can be related to diffusion. To escape the system a particle needs to have a mean squared displacement of $\left(\frac{L}{2}\right)^2$. In the program there is the ability to record particle lifetimes, can you modify the program to save the particle lifetimes and output them to a file and then estimate the diffusion coefficient?

To investigate a subtlety of the model try altering the left and right hopping rates so they are asymmetrical, a very slight change will heavily alter the escape numbers. Now reset the rates to be equal and change the energy of the sites to be sloped. This will have the same effect on escape numbers, but as a subtle point what is the difference in the physical process underlying it?

2 3D Model

This is now a more realistic three dimensional model. The energy scale is now real, the temperature is in Kelvin and charges are measured in Coulombs. N.B. *there are two values of k_B, one is in Joules, one in electron-volts. Make sure you can use the right units, as a rule the energies that are for charged particles (HOMO, LUMO and Coulomb interactions are in eV).* The program outputs the current density and simulation time in the outputs file. To record a $J-V$ curve you can run the simulation at several different net biases and plot the figure.

By changing the mobility of the electrons and holes you can alter the current densities from the device, similar to increasing the rate of incoming photons. In fact there are many changes that will manifest in the current density, it is a rather inexact measurement at this scale really. Instead let us take advantage of the resolution we have at this scale, as for the 1D case the program records particle lifetimes. Output these to a file and plot the typical lifetimes of electrons and holes, for equal parameters they will be the same.

At the moment the HOMO and LUMO levels of the materials are perfectly flat. In reality we expect there to be disorder in the energy levels, most simply modelled as a Gaussian variation. There are two parameters in the simulation that describe the disorder in the n-type and p-type materials. In the `load_morphology`function there is a loop that applies the net bias on the device to the energy levels, exactly as for the 1D case. Now the loop is extended so that it also applies a small change in the energy level drawn from a Gaussian distribution with the relevant σ value.

What effect does the disorder have on the results of the simulation? By making the disorder in the two material quite different examine the change in J and the lifetimes.

Alternatively you could add trapping defects to the simulation. A defect is represented as a site with a single energy level that is lower than the LUMO level energy and higher than the HOMO level, such that charge carriers are extremely unlikely to escape. This is usually expressed in terms of the defect density, that is the number of defects per lattice site (must be < 1).

Now you could examine the effect of morphology, load the interdigitated morphology by supplying `kmc_main.py` with the relevant filename "`DIGITATED` ". Look at the resulting output files, specifically the number of singlet disassociations compared to the number of singlet decays.

If you have the time and are interested the model can be extended. Initially the absorption of photons is homogenous throughout the entire device. The next simplest method is to consider light attenuation through the device and modify the singlet generation probability with Beer's law.