README.md

afm-sim (HoppingDynamics engine in SiQAD)

Hopping dynamics simulation and animation for silicon dangling bond devices.

Hopping Model Animator

Interactive simulation of the surface charge configurations. Charge dynamics are simulated using Hopping rate calculation from a choice of Hopping Models.

Main Functionality

- Approximately real time simulation of surface configurations.
- Control of certain physical and modeling parameters (see **Options Panel** below).
- Automatic population control through surface-bulk(reservoir) hopping.
- Placement of doubly occupied perturbers during simulation.
- Integration of a simple STM tip model (**In Progress**)
- Clocking field generation.

Keyboard shortcuts:

Key	Behaviour
Q	Close the animator (and compile the recording if enabled)
O	Open the options panel
P	Pause animation
T	When clocking, start a timer which automatically pauses the animation after a quarter phase.
S	Timestamped .png screenshot of display window (no sidepanel) to local directory
Shift + S	Timestamped .svg/.pdf screenshot of display window with capture presets.
Space	Advance the simulation one time step, somewhat deprecated.
-	Zoom out
+ or **=**	Zoom in
E	Zoom extents
L	Start line-scan at current dimer row if tip channel included.
D	Detach GUI hook for Debug

Mouse Commands

Button	Behaviour
Left Click	Clicking any hydrogen site will add/remove a fixed charge at that location.
Right Click	Right clicking a DB will track its local potential on the options dialog. Re-click the same DB or a hydrogen site to end the tracking.
Middle Click	Panning

Control + Wheel	Zoom anchored at cursor.

Tip Paths

If the tip is enabled (see **Tip Properties** in **Options Panel** below), you are able to specify paths for the tip to follow. When first created, the tip will appear at the origin of the scene coordinates. Holding shift and left clicking will cause the tip to move to the clicked position at the current tip scan rate (changeable under **Tip Properties**).

There are currently two programmed paths:

1. **Line Scan**: The **L** shortcut or **Line** button will start a line scan along the x axis that is as wide as your full device plus the **Padding**. This scan will occur on the nearest dimer row to the initial tip position.
2. **Full Scan**: The **Full** button will perform a 2D raster scan over a rectangle containing the full device plus **Padding** on each side. The tip will device this region into **Lines** line scans.

These paths, and the manual paths described below, repeat. To stop the tip, you currently have to shift click.

Creating paths

If you hold control while shift clicking, it indicates a node along a multi-node path. You can continue to shift click, holding the control key, for as many points as you like. Once control is released, the tip will begin to trace the specified path.

Options Panel

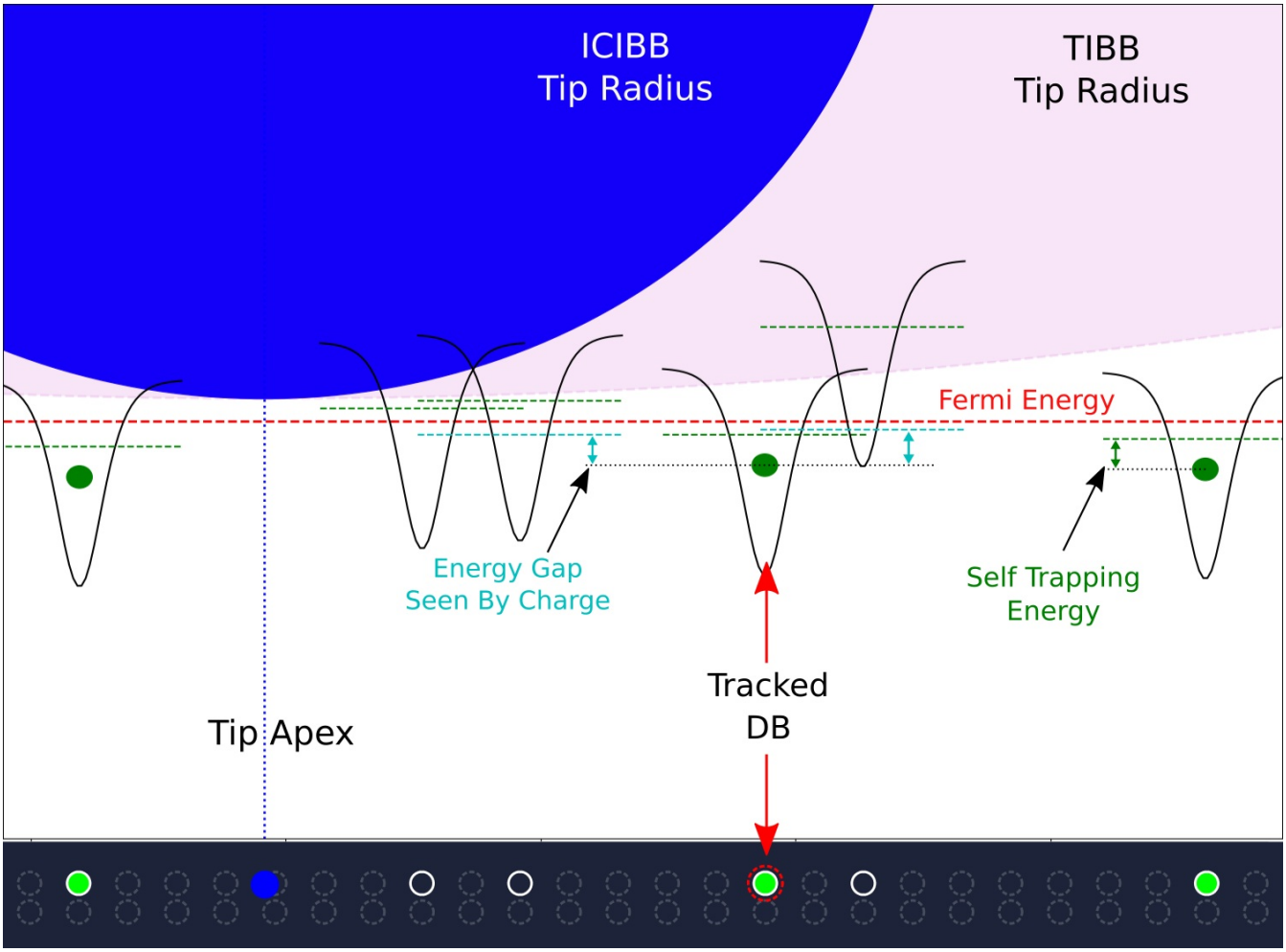
The options panel offers a selection of parameter controls/views for debugging purposes. Details of slider controls can be found in the hover tooltips.

NOTE: Currently, the sliders in the options panel only update the simulation values when the handle is released by the mouse. Using the keyboard or clicking elsewhere on the slider may not correctly update the values. Fix that soon.

Field	Context
DB-Beff	Local potential experience by targetted DB, see **Right Click** behaviour
Lifetime	Countdown for tracked DB. When the countdown runs out, the occupying charge will hop.
# electrons	Current number of electrons in the surface DBs.
Runtime Load	Percentage of time between frames used for simulating the surface state. If greater than 100%, the animation is no longer running in real time.
	Animation Controls
Viewer	See below
log(rate)	Changes the time step of the animator by 10^rate
	Hopping Model
lambda	Self trapping energy. At lambda=0, hopping models are calibrated to match the 1-2-2-1 results.
factor	Hopping rates are multiplied by 10^factor. Use instead of **rate** to increase just the hopping rates.
FRH	To increase performance, hops are only allowed within a certain range and cohopping only allowed from occupied DB pairs within a certain range. The FRH parameters change this range.
	Bulk Properties

mu	Chemical potential for utomatic population mechanism. This is effectively the energy difference between the Fermi level and the DB- state of an isolated DB.
	Tip Properties
Tip	If the Tip channel is included in the Hopping model, "Tip properties" and "Tip programs" will be available in the options
scale	Scales the tip influence, TIBB and ICIBB. Tip seems to be fairly well behaved for scale < 0.3 or so.
epsr	Relative permittivity for Coulomb interactions between DBs and image charges. Lower epsr will make ICIBB stronger
H	Tip height above the surface, in pm
ICIBB R	Tip radius for ICIBB (image charge localised near the point of the tip)
TIBB R	Tip radius for TIBB (blunt tip with long range contact potential influence)
rate	Tip scanning speed
	Tip Programs
Padding	Extra space added to the outside of line and full (2D raster) scans
Lines	Number of lines/rows in the full scan
Line	Start a line scan horizontally along the nearest row of atoms.
Full	Scan the tip over a region containing the full device.
	Clocking Field
Clocking	If the Clocking channel is incuded in the Hopping model, "Clocking Field" will be available in the options. The clock is a sinusoidal potential that travels to the right and effectively shifts the DB- level.
Frequency	Frequency of the clocking field
Amplitude	Amplitude of the clocking field, in eV
Offset	Offset of the clocking field, essentially equivalent to more **mu**
Flat Clock	Currently broken: essentially sets the wavelength to infinite.

Viewer



The Viewer is an additional tool which shows a representation of the device (currently collapsed onto the x axis). A well is drawn for each well with the black line indicating the energy of the DB- state and the green dots showing the current charge locations. For significant **lambda**, the dots will be noticeably lower than the DB- levels to indicate the self-trapping. If a DB is being tracked (see **Right Click** behaviour), blue lines will be shown for the possible hopping targets which indicate the effective energy level seen by the tracked charge. The tip will be shown if included with both radii shown and the apex indicated. *Clearly insert figure here*.

Current Bugs

If there are ever fewer than 2 free DBs the cohopping implementation will throw an Error. *Edit: 2018.05.02 Not sure if this still happens*