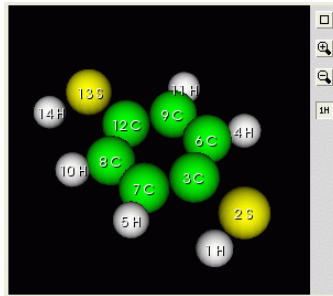


Advanced Rappture Concepts

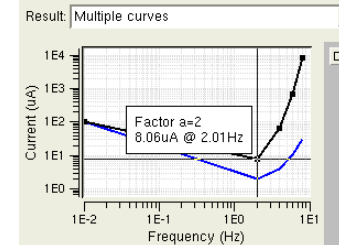


Carrier Statistics:

- Boltzmann
- Fermi
- 2D Gas

Grid points:

Ambient temperature:



Michael McLennan
Software Architect
HUBzero™ Platform for Scientific Collaboration

Identify the elements

<group> of <group>'s

<choice>

<group>

<number>

<structure>

<box>

<field>

PN Junction Lab (v. 1.1padre)

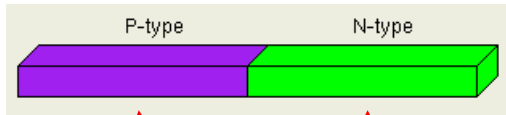
Learn about any kind of P(I)N junction as you explore the devices in this simulator.

Input values for the various parameters on the left and click "Simulate" at the top to run the simulation. The parameters are currently set to model a standard PN junction diode. (no intrinsic region)

- Material Properties
Define the material properties of the device, including elements and carrier lifetimes.
- Structural Properties
Define the dimensional properties of the device, as well as the sample points taken along those dimensions.
- Temperature and Voltage
Set the ambient temperature and voltage sweep parameters.
- Doping
Set the amount for doping for both P and N type materials. (Note: Intrinsic region always has zero doping)

<structure>

Structure of physical system being simulated



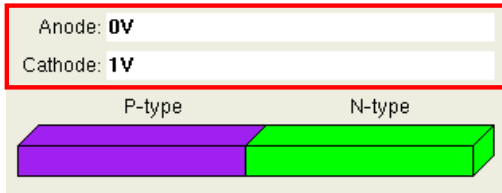
Just 1-D boxes,
for now

```

<structure>
  <current>
    <components>
      <box>
        <about>
          <label>P-type</label><color>purple</color>
        </about>
        <corner>0</corner>
        <corner>0.1um</corner>
      </box>
      <box>
        <about>
          <label>N-type</label><color>green</color>
        </about>
        <corner>0.1um</corner>
        <corner>0.2um</corner>
      </box>
    </components>
  </current>
</structure>
  
```

<structure>

Structure of physical system being simulated

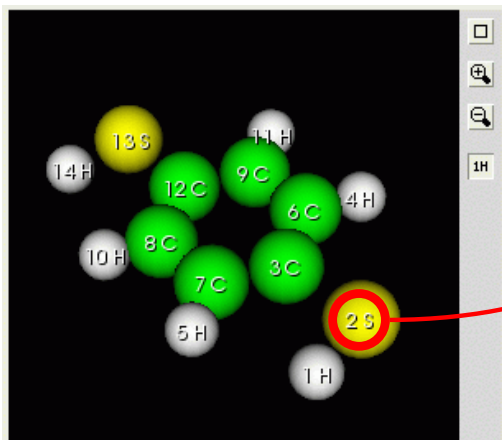


```

<structure>
  <current>
    <parameters>
      <number>
        <about><l a b e l >Anode: </l a b e l ></about>
        <u n i t s>V</u n i t s>
        <d e f a u l t>0V</d e f a u l t>
      </number>
      <number>
        <about><l a b e l >Cathode: </l a b e l ></about>
        <u n i t s>V</u n i t s>
        <d e f a u l t>1V</d e f a u l t>
      </number>
    </parameters>

    <components>...</components> ——— Same as before
  </current>
</structure>
  
```

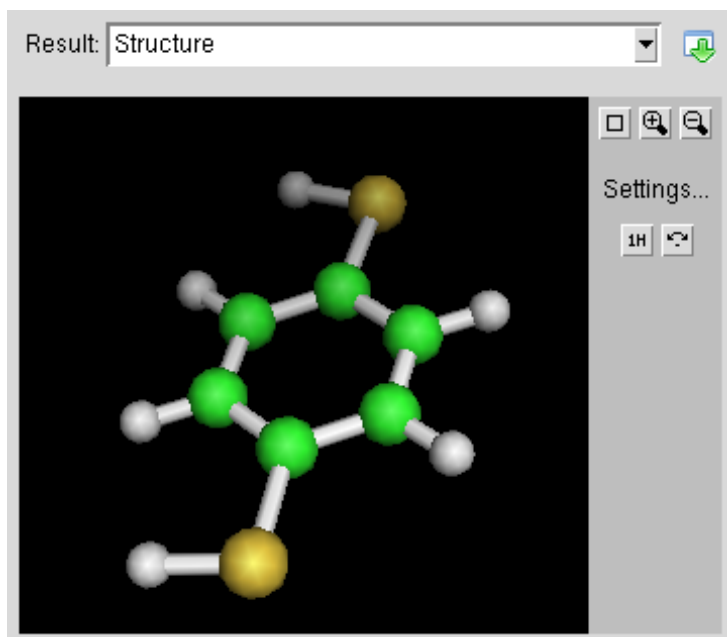
<structure>

Molecule as input parameter

Turns atom labels
on by default

```
<structure>
  <current>
    <components>
      <mol ecul e>
        <about><embl ems>on</embl ems></about>
        <formul a>pdt</formul a>
        <atom i d="0">
          <symbol >H</symbol >
          <xyz>-1.24935 -3.41562 0.0</xyz>
        </atom>
        <atom i d="1">
          <symbol >S</symbol >
          <xyz>0.08092 -3.19426 0.0</xyz>
        </atom>
        ...
      </mol ecul e>
    </components>
  </current>
</structure>
```

<structure>

Molecule produced as output

```
import Rappture
import sys
driver = Rappture.Library(sys.argv[1])
...
path = 'output.structure(mol)'
driver.put(path+'.about.label', 'Structure')

path += 'components.molecule'
driver.put(path+'.atom(0).symbol', 'H')
driver.put(path+'.atom(0).xyz', xyz0)
driver.put(path+'.atom(1).symbol', 'S')
driver.put(path+'.atom(1).xyz', xyz1)
...
```

<sequence>

Sequence of images, curves, or fields



```

<sequence id="movie">
  <about>
    <label>Animated sequence</label>
  </about>
  <index><label>Frame</label></index>

  <element id="0">
    <index>1</index>
    <image>
      <current>/9j/4AAQSkZJRgAA...</current>
    </image>
  </element>

  <element id="1">
    <index>2</index>
    <image>
      <current>/9j/4ARgASkZJQQR...</current>
    </image>
  </element>

  ...
</sequence>

```

Just like a normal output image

Describe everything

What are these two parameters?

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42A

- Good descriptions say:
- What the parameter means
 - Typical value or range
 - What happens at 0 or min
 - What happens at ∞ or max

```
<number id="TightBindingEnergy" >
  <about>
    <label>Tight Binding Energy</label>
    <description>This is the tight binding overlap
integral, or hopping energy. It is a measure of the
overlap of orbitals in the
nanotube. Typical values are 3eV.
References on details. </desc
...

```

Rappture generates this part automatically

n: 7

m: 7

Model parameters

Tight Binding Energy: 3eV

Carbon-carbon spacing: 1.42A

Length in 3-D view: 15

This application is powered by: Octave, Matlab and 77. Last updated November 2006.

For nanotubes, try n=7, m=7 (7,7) to see an "armchair" metallic nanotube. Then try a (12,0) "zigzag" nanotube which is a different kind of metallic nanotube. Next, (13,0) zigzag nanotube. The energy gap in the band structure is 0.1 eV for (7,7), 0.2 eV for (12,0), and 0.3 eV for (13,0).

This is the distance between the centers of any two carbon atoms in the nanostructure. Usually 1.42A, but you can adjust it if you don't believe the usual value.

Enter a number between 1.3A and 1.5A with units of length (A,m)

Describe EVERYTHING

You can add <description>'s to...

- All inputs
- All outputs
- <option> within a <choice>
- <group>
- Examples accessed through <loader>
- <xaxis> and <yaxis> with a <curve>

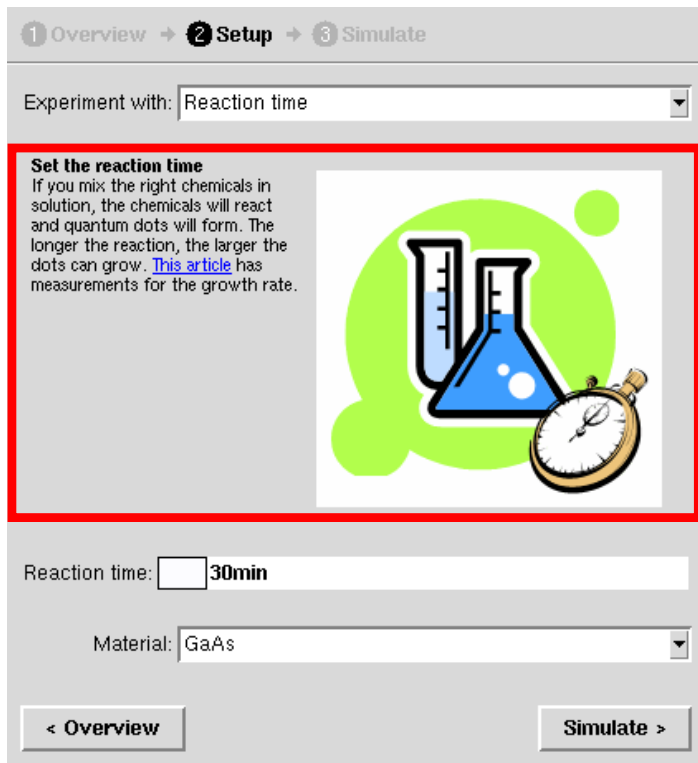
The screenshot shows a software interface with several callout boxes:

- Minority carrier lifetimes:** Groups can be used two ways normally drawn with a gray background. Majority carriers are the same as the doping type--either p-type or n-type. Minority carriers are the opposite of the majority type. Minority carriers often live for a short time before being lost to recombination events. These parameters set the lifetime.
- Carrier Statistics:** Boltzmann. When you click the Simulate button used to generate the output choice. Determines the model for carrier statistics used in bandgap narrowing calculations. Boltzmann: From the Boltzmann transport equation.
- Example:** Change both. Use this to load examples. Change both: This example changes both inputs, #1 to "first" and #2 to "second". Example of a Rabbure <loader> object.
- Result:** Extinction Cross Section. Extinction is the sum of scattering and absorption. It is a measure of how much light is removed from the incident beam. Use this control to display other output results.
- Extinction efficiency:** Extinction efficiency relative to the cross sectional area of the particle. Extinction is the sum of scattering and absorption.

The interface also features a graph with a blue curve and a 'Simulate' button.

Set the stage

Use `<note>` elements to explain your tool to the user:



- Not an input
- Descriptive text for the user
- Full HTML support

```
<i nput >
  <note>
    <contents>file: //by size. html </contents>
  </note>
  ...
```

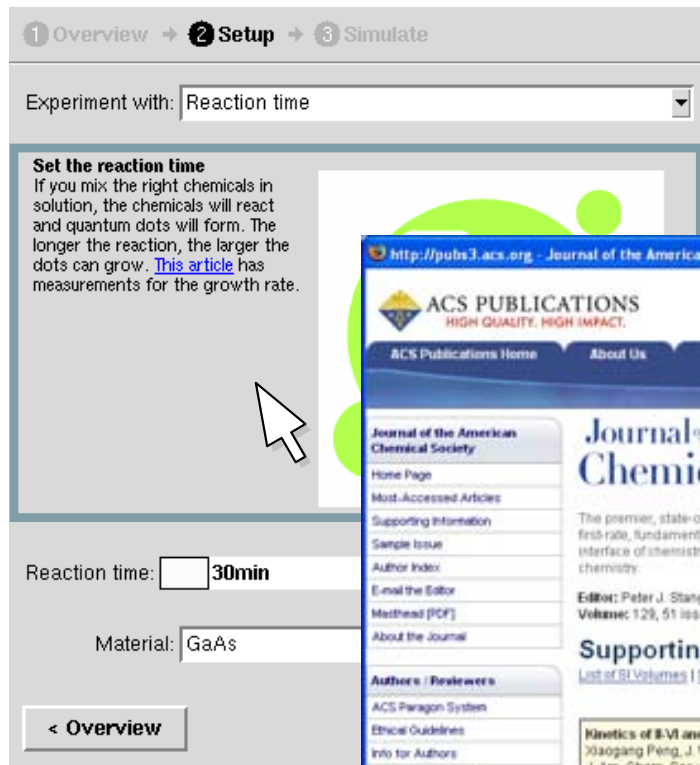
file: docs/by size. html

```
<html >
<body>
<p>

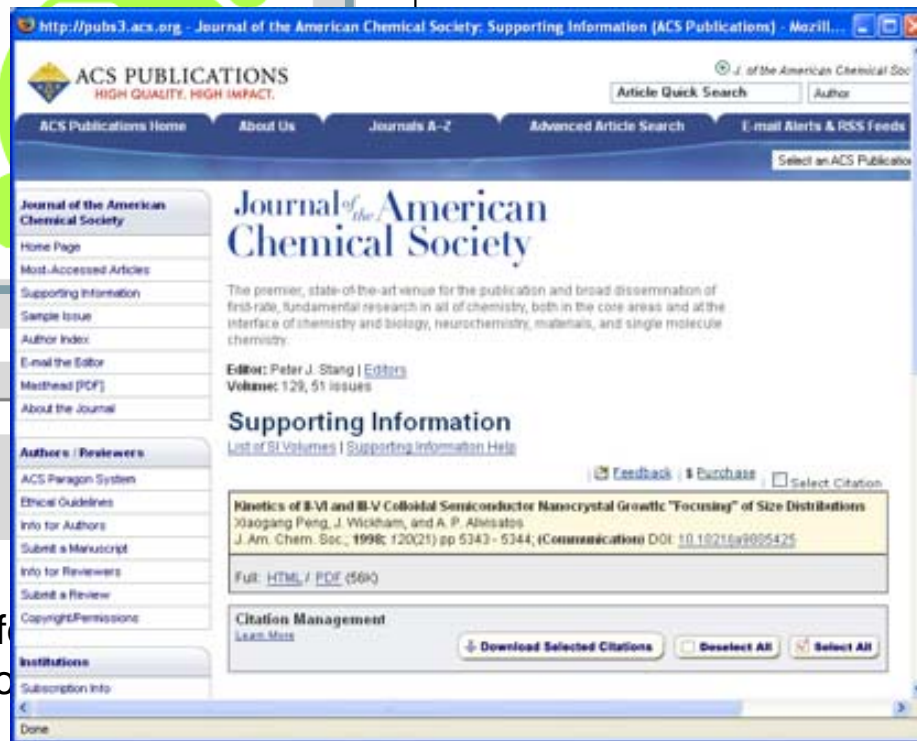
<b>Set the reaction time</b><br/>
If you mix the right chemicals in solution,
the chemicals will react and quantum dots
will form. The longer the reaction, the
...
```

Set the stage

Use `<note>` elements to explain your tool to the user:



```
<i nput>
<note>
  <contents>file://by size. html </contents>
</note>
```



- Not an input
- Descriptive text for
- Full HTML support

ml

ight; margin: 8px; "

time

chemicals in solution,
react and quantum dots
er the reaction, the

Tour the zoo

rappture_xml_elements - Rappture - Trac - Mozilla Firefox

https://developer.nanohub.org/projects/rappture/wiki/rappture_xml_elements

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Zoo of Inputs/Outputs

Welcome to the zoo of Rappture elements! This page shows the various snippets of XML code needed to create a Rappture tool.xml file.

Overall Structure

Each tool is described by a tool.xml file, which has the following structure:

```
<?xml version="1.0"?>
<root>
  <tool>
    <title>Name of the tool</title>
    <about>Description and credits</about>
    <command>
      @tool/path/to/executable @driver
    </command>
    <limits>
      <cpulimit>900</cpulimit>
      <filesize>1000000</filesize>
    </limits>
    <layout>xxx</layout>
    <control>xxx</control>
    <analyser>xxx</analyser>
    <reportJobFailures>1</reportJobFailures>
  </tool>
  <input>
    ...see Element Index below...
  </input>
  <output>
    ...see Element Index below...
  </output>
</root>
```

The <tool> section describes the underlying compute engine and includes the command needed to run it. This can be any Unix-style command line. The @tool keyword gets replaced with the name of the directory containing the tool.xml file. The

Carrier Statistics: Fermi

Boltzmann

Fermi

2D Gas

Ambient temperature: 300K

Grid points: 100

Zoo of Examples

- Complete catalog of data objects online
- See screen shots
- Copy xml code

Exercise #5: Add notes to Spirograph

Add a note with overview.html text

Extra Credit: Include an image and a hyperlink

Fun with Spirographs

The spirograph equations for three or more wheels can be generalized as follows:

$$z(t) = \sum_{k=1}^n a_k e^{i2\pi(n_k t + \theta_k)}, \quad t \in [0, 1],$$

This program solves those equations for three wheels, assuming all of the a and θ coefficients are 0. Find more details online at <http://linuxgazette.net/133/auana.html>.

Model Parameters Comments

n1: **13**

n2: **-7**

n3: **-3**

Simulate

Result: Spirograph

1 result Parameters... Clear