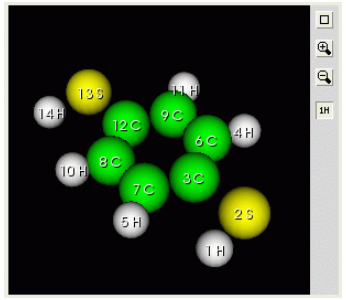
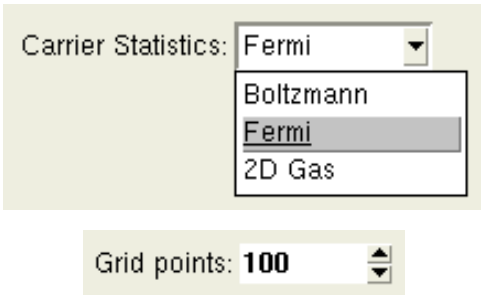
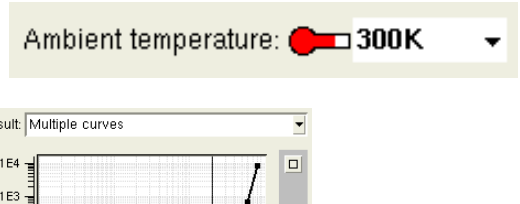
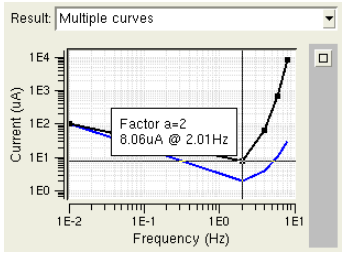
Advanced Rappture Concepts









Michael McLennan
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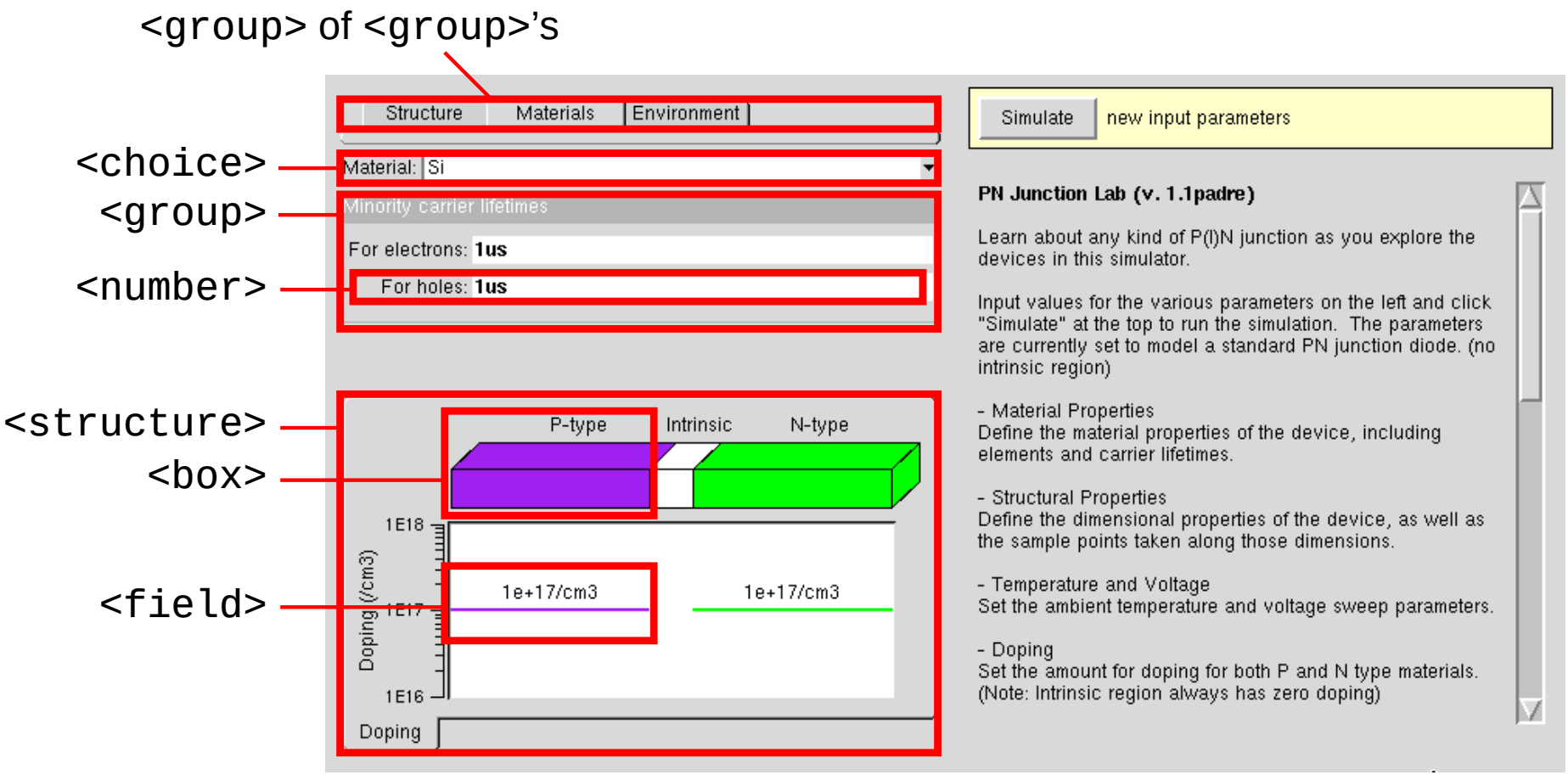
HUBzero™ Platform for Scientific Collaboration

Identify the elements



<structure>

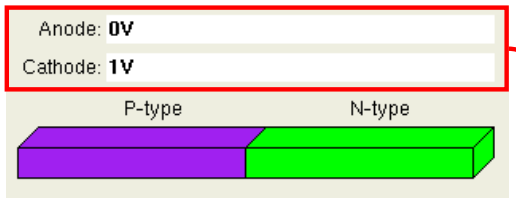
Structure of physical system being simulated

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



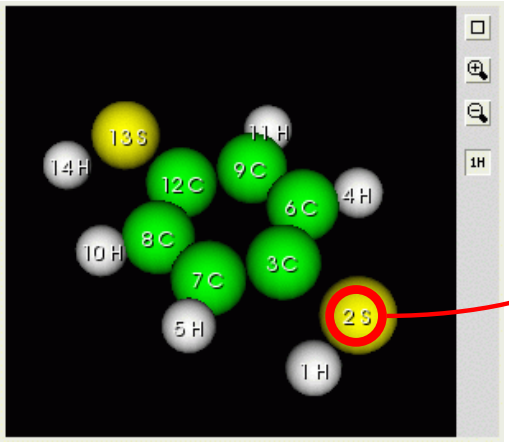

```
<structure>
  <current>
    <parameters>
      <number>
        <about><label>Anode:</label></about>
        <units>V</units>
        <default>0V</default>
      </number>
      <number>
        <about><label>Cathode:</label></about>
        <units>V</units>
        <default>1V</default>
      </number>
    </parameters>

    <components>…</components>
  </current>
</structure>
```

Same as before

<structure>

Molecule as input parameter

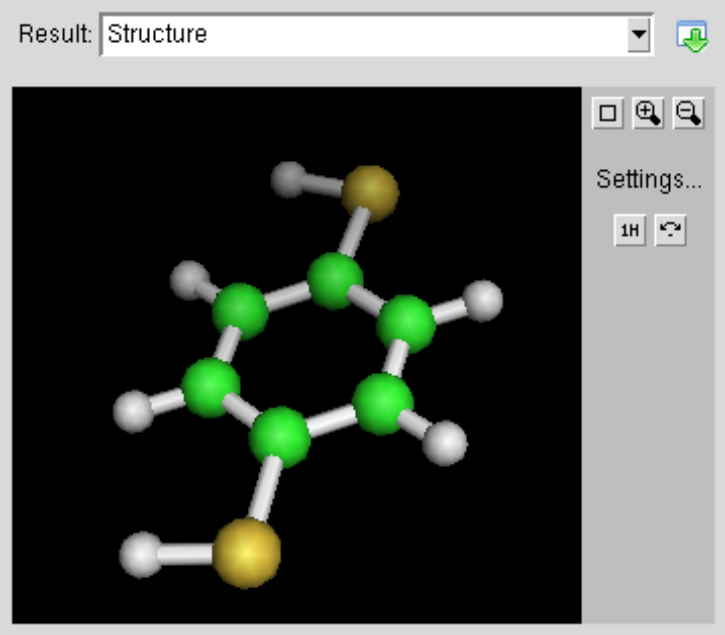


Turns atom labels on by default

```
<structure>
  <current>
    <components>
      <molecule>
        <about><emblems>on</emblems></about>
        <formula>pdt</formula>
        <atom id="0“>
          <symbol>H</symbol>
          <xyz>-1.24935 -3.41562 0.0</xyz>
        </atom>
        <atom id="1">
          <symbol>S</symbol>
          <xyz>0.08092 -3.19426 0.0</xyz>
        </atom>
        …
      </molecule>
    </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

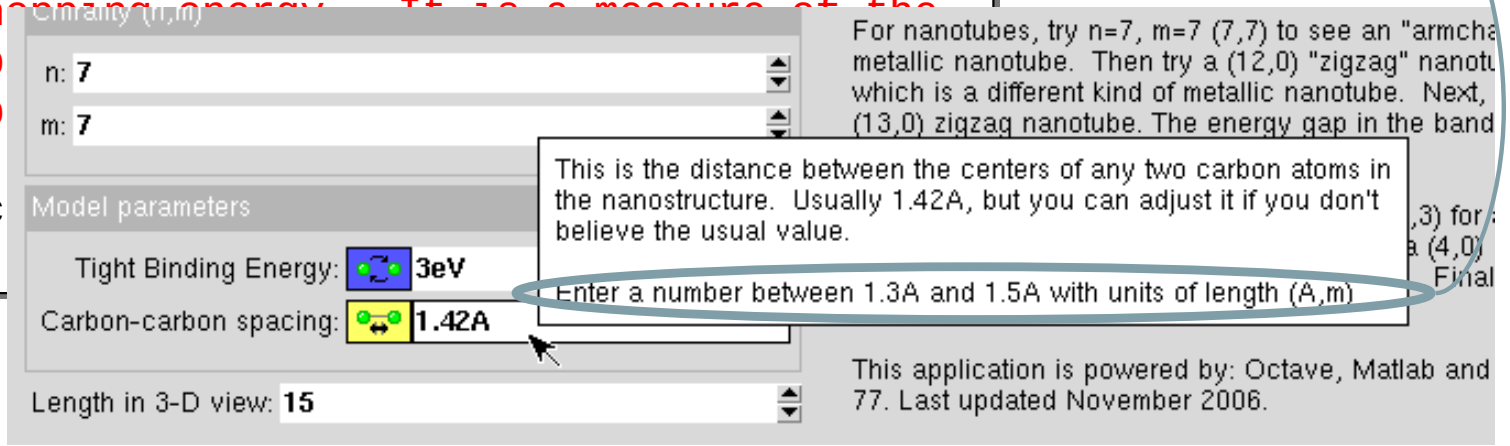
What are these two parameters?

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 orb
nanotube.  Typ
references on
details.</desc
    ...
```

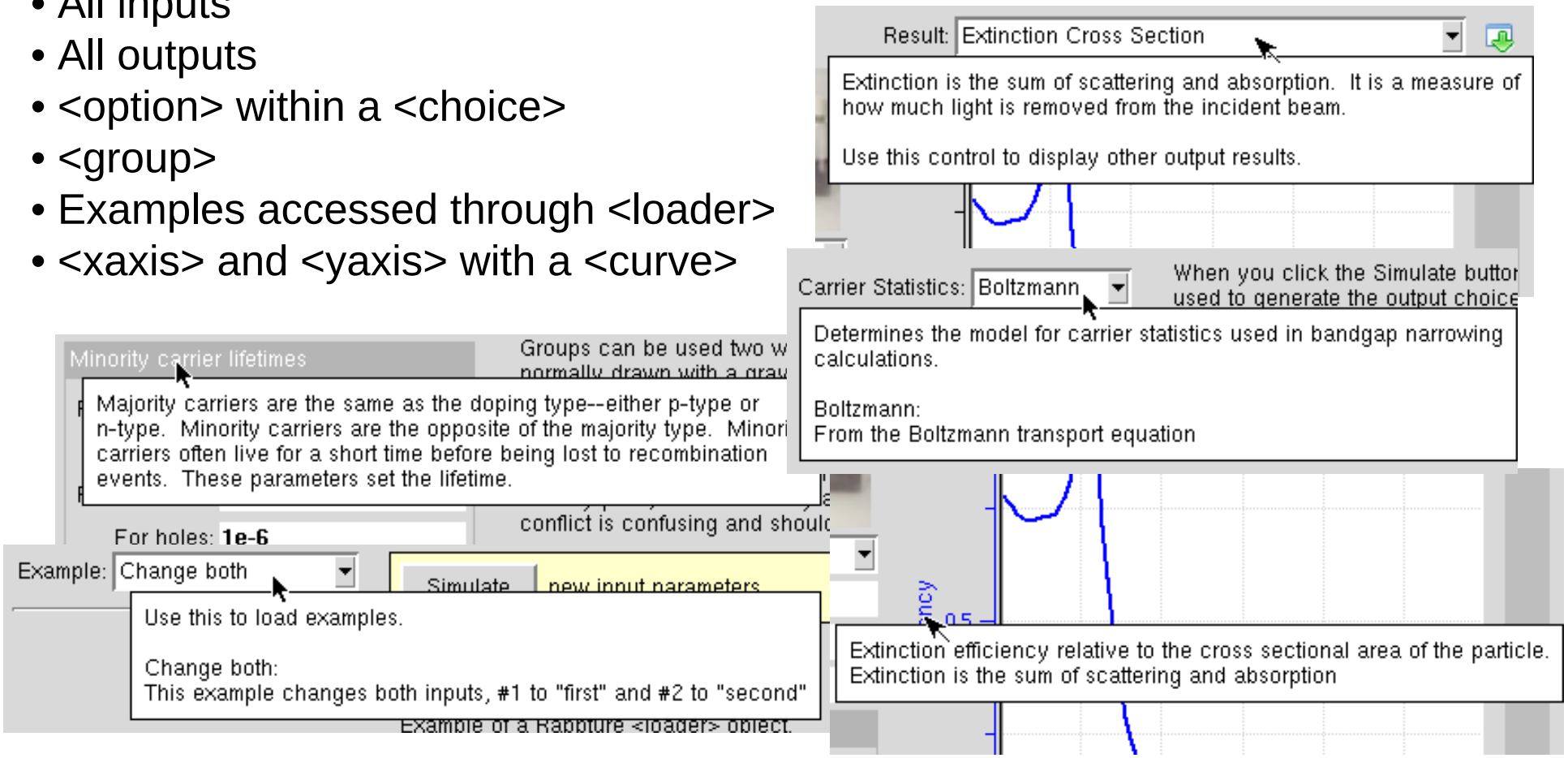
Rappture generates this part automatically



Describe EVERYTHING

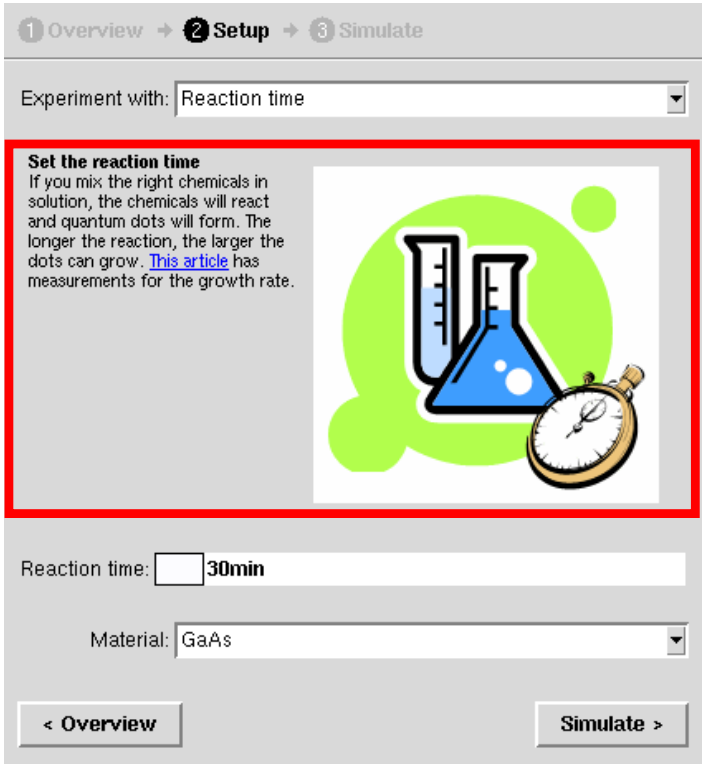
You can add <description>'s to...

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



Set the stage

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



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

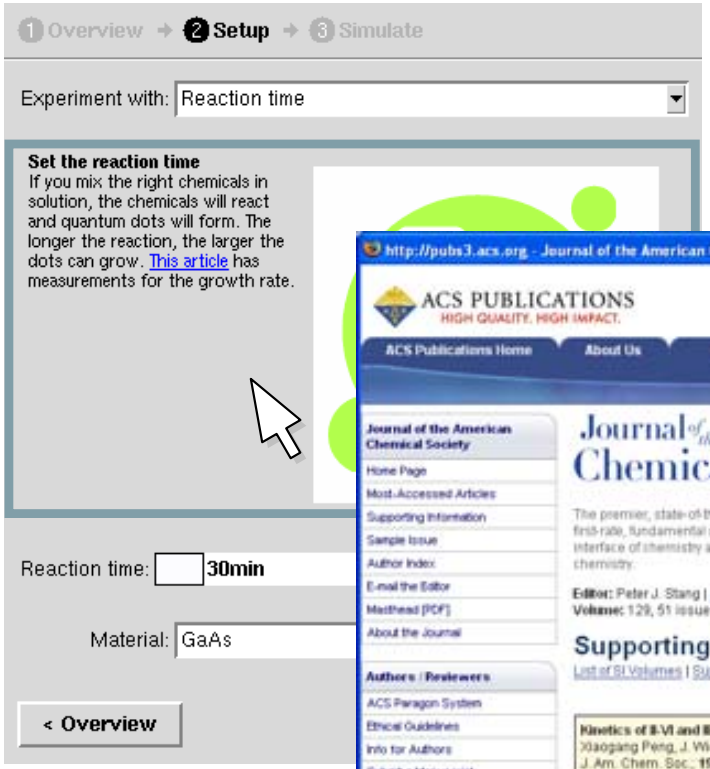
```
<input>
  <note>
    <contents>file://bysize.html</contents>
  </note>
  …
```

file: docs/bysize.html

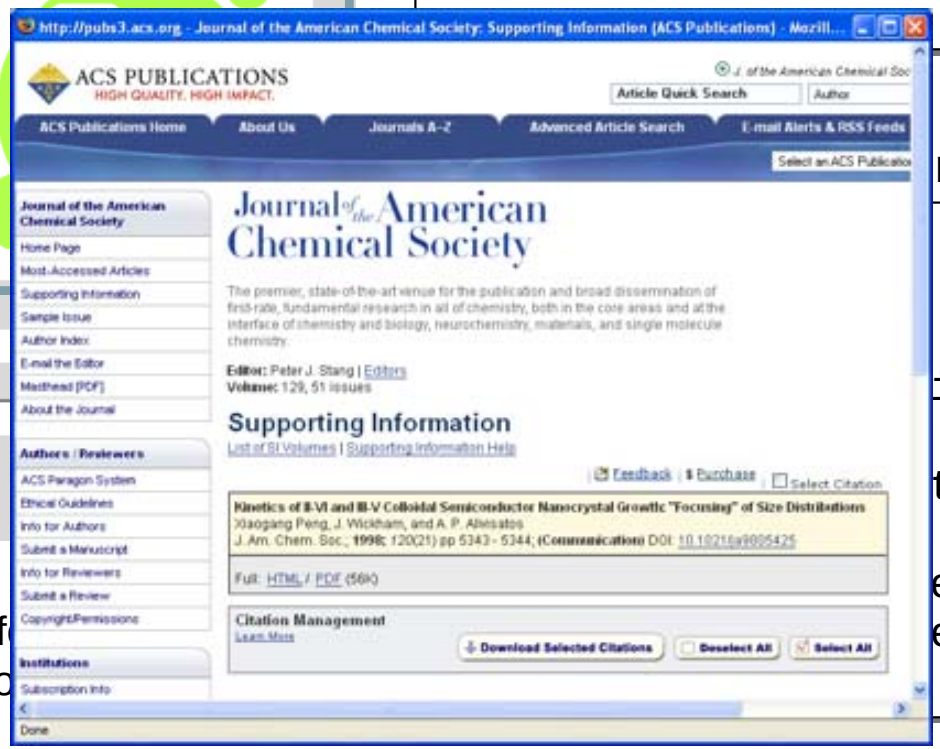
```
<html>
<body>
<p>
<img style="float: right; margin: 8px;"
src="bytime.gif"/>
<b>Set the reaction time</b><br/>
If you mix the right chemicals in solution,
the chemicals will react and quantum dots
will form.  The longer the reaction, the
…
```

Set the stage

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




```
<input>
  <note>
    <contents>file://bysize.html</contents>
  </note>
```



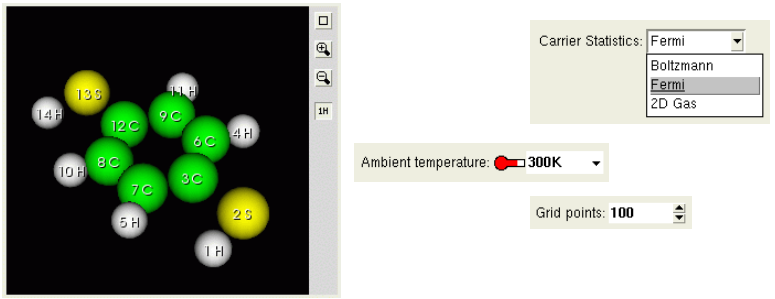

```
ml

ight; margin: 8px;"

time</b><br/>
 chemicals in solution,
eact and quantum dots
er the reaction, the
```

- Not an input
- Descriptive text f
- Full HTML suppo

Tour the zoo



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