



More Rappture Objects

Michael McLennan

*HUBzero® Platform for Scientific Collaboration
Purdue University*

This work licensed under
Creative Commons



See license online:
by-nc-sa/3.0



Use Group objects to group inputs together

Tool Interface:

Tool:

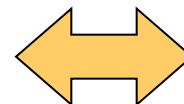
+ Input:

+ Group: tau

Number: taun

Number: taup

+ Output:



Minority carrier lifetimes

For electrons: **1e-6**

For holes: **1e-6**

Object: input.group(tau) Rename

Help Delete

Label: Minority carrier lifetimes

Average time that it takes for a minority carrier to recombine, releasing energy in the form of phonons or photons.

Description:

Add label/description to groups

Minority carrier lifetimes

Average time that it takes for a minority carrier to recombine, releasing energy in the form of phonons or photons.



Group of Groups

Tool Interface:

Tool:

+ Input:

+ Group: tabs

+ Group: models

Boolean: recomb

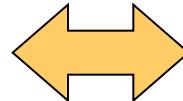
+ Group: tau

Number: taun

Number: taup

+ Group: ambient

Number: temp



Models Ambient

Recombination Model: yes

Minority carrier lifetimes

For electrons: **1e-6**

For holes: **1e-6**

Models Ambient

Temperature: **300K**

Group of just groups \Rightarrow tabs _____

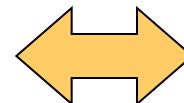
Group with other elements \Rightarrow box with group contents _____



Use Phase objects to create input panels

Tool Interface:

Tool:
⊕ Input:
 ⊕ Phase: one
 String: first
 ⊕ Phase: two
 String: second



The screenshot shows a two-page input process. The top part is labeled "First Page" and contains a text input field with the value "one". The bottom part is labeled "Second Page" and contains a text input field with the value "two". Both pages have navigation buttons: "First Page" and "Simulate".

1 First Page → 2 Second Page → 3 Simulate

First input: one

Second Page >

1 First Page → 2 Second Page → 3 Simulate

Second input: two

< First Page Simulate >

* Use this sparingly--only if there are already lots of inputs and groups.



Use Enable condition to enable/disable inputs

Drift-Diffusion Options

Recombination Model: no

Minority Carrier Lifetime for electrons: 1e-6

Minority Carrier Lifetime for holes: 1e-6

Drift-Diffusion Options

Recombination Model: yes

Minority Carrier Lifetime for electrons: 1e-6

Minority Carrier Lifetime for holes: 1e-6

boolean
enables/disables
number entries

Tool Interface:

Tool:
+ Input:
 Choice: model
 + Group: dd
 Boolean: recomb
 Number: taun
 Number: taup
 + Group: bte
 Number: temp
 Integer: secret
 + Group: negf
 Number: the

Object: `input.group(dd).boolean(recomb)` Copy

Label: Recombination Model

Tool Interface:

Tool:
+ Input:
 Choice: model
 + Group: dd
 Boolean: recomb
 Number: taun
 Number: taup
 + Group: bte
 Number: temp
 Integer: secret
 + Group: negf
 Number: the

Object: `input.group(dd).number(taun)` Rename

Label: Minority Carrier Lifetime for electrons

Description:

Enable: `input.group(dd).boolean(recomb)`

Default Value: 1e-6

2

Paste (ctrl-Y)
into the Enable
condition of each
number

1

Copy the path for the boolean



Enable condition can be an expression

Quantum Mechanical Options

Tight-binding Energy: **2.99eV**

High-energy lifetime: **10ns**

Quantum Mechanical Options

Tight-binding Energy: **3.01eV**

High-energy lifetime: **10ns**

number value
enables/disables
number below it

Tool Interface:

- Choice: model
- + Group: dd
 - Boolean: recomb
 - Number: taun
 - Number: taup
- + Group: bte
 - Number: temp
 - Integer: secret
- + Group: negf
 - Number: tbe
 - Number: tau
- + Output:
 - Object: input.group(negf).number(tau) Rename
 - Label:** High-energy lifetime
 - Description:** This is used only when the tight-
 - Enable:** input.(negf).(tbe):eV >= 3
 - Default Value:** 10ns

Get the value of the
tight-binding energy
number

Convert
to eV

i nput. (negf) . (tbe) : eV >= 3

Enable High-energy lifetime
whenever $tbe \geq 3$



Use Enable condition to enable/disable whole groups

Model: Drift-Diffusion

Drift-Diffusion Options

Recombination Model: no

Minority Carrier Lifetime for electrons: 1e-6

Minority Carrier Lifetime for holes: 1e-6

Group

Enable: `input.choice(model) == "dd"`

Model: Boltzmann Transport Equation

Boltzmann Transport Equation Options

Temperature: 300K

Group

Enable: `input.choice(model) == "bte"`

Model: Quantum Mechanical NEGF

Quantum Mechanical Options

Tight-binding Energy: 3.12eV

High-energy lifetime: 10ns

Group

Enable: `input.choice(model) == "negf"`



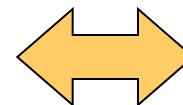
Use Note objects to embed documentation

Tool Interface:

Tool:
+ Input:
 Note: note
 Number: diameter
 Integer: num
+ Output:

Object: input.note(note) Rename Help Delete

HTML File: <file:///docs/bysize.html>



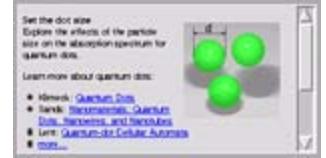
Set the dot size
Explore the effects of the particle size on the absorption spectrum for quantum dots.

Learn more about quantum dots:

- Klimeck: [Quantum Dots](#)
- Sands: [Nanomaterials: Quantum Dots, Nanowires, and Nanotubes](#)
- Lent: [Quantum-dot Cellular Automata](#)
- [more...](#)

Particle diameter d: **5nm**

Number of particles: **3**



Set an ordinary HTML file

Color xterm

```
$ ls
docs/ note.tcl tool.xml
$ ls docs
bysize.gif bysize.html
$
```

Can reference images and other HTML files in the same directory, or using absolute http:// paths



Note can pop up external web sites

Example: *bysize.html*

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

<b>Set the dot size</b><br/>
Explore the effects of the particle size on
the absorption spectrum for quantum dots.
</p><p>
Learn more about quantum dots:
<ul style="margin: 0px; padding-left: 16px;">
<li>Klimeck: <a href="http://www.nanohub.org/resources/189">Quantum Dots</a></li>
<li>Sands: <a href="http://www.nanohub.org/resources/376">Nanomaterials: Quantum Dots, Nanowires, and Nanotubes</a></li>
<li>Lent: <a href="http://www.nanohub.org/resources/148">Quantum-dot Cellular Automata</a></li>
<li><a href="http://www.nanohub.org/resources/tags/quantumdots">more...</a></li>
</ul>
</p>
</body>
</html>
```

Set the dot size
Explore the effects of the particle size on the absorption spectrum for quantum dots.

Learn more about quantum dots:

- Klimeck: [Quantum Dots](http://www.nanohub.org/resources/189)
- Sands: [Nanomaterials: Quantum Dots, Nanowires, and Nanotubes](http://www.nanohub.org/resources/376)
- Lent: [Quantum-dot Cellular Automata](http://www.nanohub.org/resources/148)
- [more...](#)

Particle diameter d:

Number of particles:

nanoHUB.org - Resources: Nanomaterials: Quantum Dots, Nanowires and Nanotubes - Google Chrome

nanoHUB.org - Resources: Nanomaterials: Quantum Dots, Nanowires and Nanotubes

ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

You are here: Resources > Online Presentations > Nanomaterials: Quantum Dots, Nanowires and ... About

Nanomaterials: Quantum Dots, Nanowires and Nanotubes

View Presentation (SWF)

By Timothy D. Sands
Purdue University

What is a quantum dot? What is a nanowire? What is a nanotube? Why are these interesting and what are their potential applications? How are they made? This presentation is intended to begin to answer these questions while introducing some ...

About Reviews Supporting Docs

Abstract: What is a quantum dot? What is a nanowire? What is a nanotube? Why are they interesting and what are their potential applications? How

SEE ALSO

Part of NCLT Seminar Series

Part of NCN Nanomaterials Tutorials

Part of Introductory Seminars



The builder is great, but it's not perfect

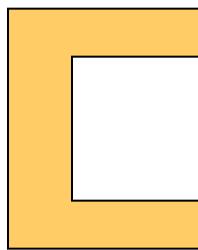
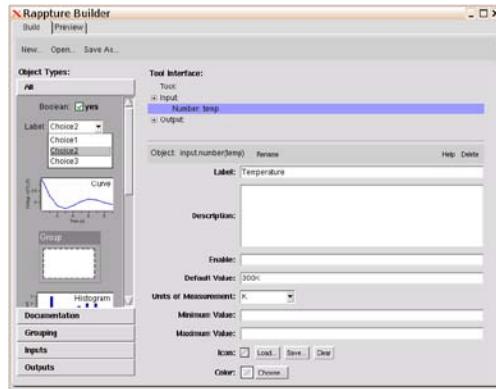
The image shows two side-by-side windows. On the left is a web browser displaying a nanoFORGE wiki page titled 'rp_xml_ele_number - infrastructure'. The page content includes XML code for a 'number' object representing temperature, with preset values for 300K and 77K. On the right is the 'Rappture Builder' application window, which shows the same XML structure. In the builder, the 'Tool Interface' panel indicates an input named 'Number: temp'. The 'Object' panel shows the XML code. The 'Label' field is set to 'Temperature', and the 'Description' field is empty. The 'Enable' field contains '300K' with a dropdown menu set to 'K'. A question mark icon in the bottom right corner of the builder window is highlighted with a red box.

Where are the preset controls?

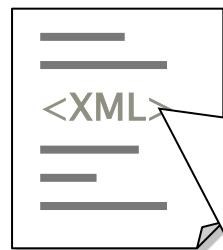


Under the hood: XML

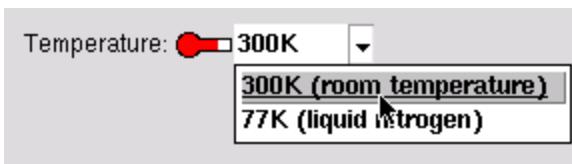
Builder



skeleton
program



tool.xml



```
<?xml version="1.0"?>
<run>
  <tool>
    <title>Example with temperature</title>
  </tool>
  <input>
    <number id="temp">
      <about>
        <label>Temperature</label>
      </about>
      <default>300K</default>
      <units>K</units>
      <preset>
        <value>300K</value>
        <label>300K (room temperature)</label>
      </preset>
      <preset>
        <value>77K</value>
        <label>77K (liquid nitrogen)</label>
      </preset>
    </number>
  </input>
</run>
```

You can add stuff
like this by hand

Prompt for elements from the periodic table

Second Element: Oxygen - O

Third Element:

1 H	2 He																
3 Li	4 Be																
11 Na	12 Mg																
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	
87 Fr	88 Ra	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uut	113 Uup	114 Uuo	115 Uup	116 Uuh	117 Uus	118 Uuo	
57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu			
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr			

actinoid
 alkali-metal
 alkaline-earth-metal
 halogen
 lanthanoid
 metalloid
 noble-gas
 other-non-metal
 post-transition-metal
 transition-metal
 unknown

<input>

```

<periodic_element id="second">
  <about> <label>Second Element</label> </about>
  <default>0</default>
  <inactive>lanthanoid actinoid</inactive>
  <returnvalue>symbol</returnvalue>
</periodic_element>
...
  
```

weight
 number
 name
 symbol
 all



Assignment #7: Add options to Spirograph

- Add a note at the very top
- Add a “model parameters” tab and a “comments” tab
- When comments are enabled, produce an output string with comments

