

Chemical Editing...

Egon Willighagen 

Published October 20, 2008

Citation

Willighagen, E. (2008, October 20). Chemical Editing... *Chem-bla-ics*. <https://doi.org/10.59350/dvb9w-vg635>

Keywords

Jchempaint, Cdk

Abstract

As you might have seen, we, Uppala and the EBI, are working on the next generation JChemPaint. JChemPaint is an editor, and therefore, consists of a model (IChemModel), a view (IRenderer) and a controller (IController). See the many posts in Gillean's blog.

Copyright

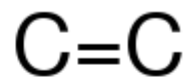
Copyright © Egon Willighagen 2008. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

chem-bla-ics

As you might have seen, we, [Uppala](#) and the [EBI](#), are working on the next generation [JChemPaint](#). JChemPaint is an editor, and therefore, consists of a model (**IChemModel**), a view (**IRenderer**) and a controller (**IController**). See the many posts in [Gilleain's blog](#).

For the renderer I have set up a [wiki page](#) which I'll be hacking in the next days, which shows how a **IChemObject** content should be rendered in JChemPaint. It looks like:

```
IAtom atom0 = builder.newAtom("C");  
IAtom atom1 = builder.newAtom("C");  
IBond bond = builder.newBond(atom0, atom1, IBond.Order.DOUBLE);
```



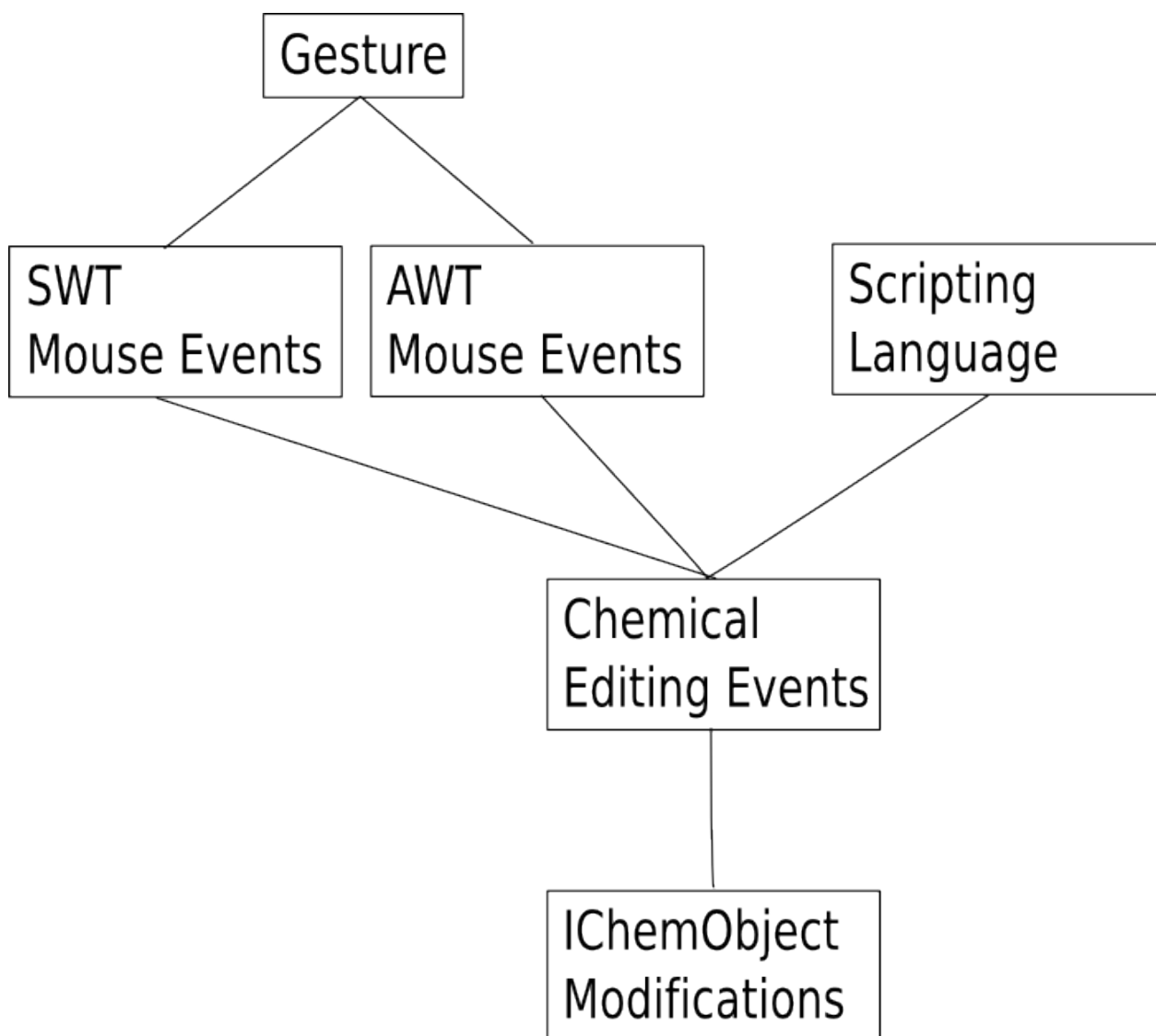
```
IAtom atom0 = builder.newAtom("C");  
IAtom atom1 = builder.newAtom("C");  
IBond bond = builder.newBond(atom0, atom1, IBond.Order.TRIPLE);
```



```
IAtom atom0 = builder.newAtom("C");  
atom0.setFormalCharge(1);
```



The **IController** is a rather important part too, and like the **IRenderer** bit of JChemPaint, needs a major overhaul. The new design, discussed by Gilleain [here](#) and [here](#), should, IMHO, look like:



In this diagram, the gestures can come from any input device, mouse, tracking ball, Wiimote, and will result in events in some widget library (SWT, AWT shown). The old JChemPaint, converted the Swing `MouseEvent`'s directly into `IChemObject` modifications, making the code incompatible with SWT. This is why the *Chemical Editing Events* layer must be added.

Events in this layer look like `addAtom(attachmentAtom, coordinates)` and `setFormalCharge(atom, newCharge)`. The link to scripting should be clear now, and will help use write unit tests for this layer.