<table>
<thead>
<tr>
<th>Title</th>
<th>Light-operated rotaxanes on graphene</th>
</tr>
</thead>
<tbody>
<tr>
<td>Author(s)</td>
<td>Li, Xing</td>
</tr>
<tr>
<td>Citation</td>
<td>Li, X. (2012, March). Light-operated rotaxanes on graphene. Presented at Discover URECA @ NTU poster exhibition and competition, Nanyang Technological University, Singapore.</td>
</tr>
<tr>
<td>Date</td>
<td>2012</td>
</tr>
<tr>
<td>URL</td>
<td><a href="http://hdl.handle.net/10220/8939">http://hdl.handle.net/10220/8939</a></td>
</tr>
<tr>
<td>Rights</td>
<td>2012 The Author(s).</td>
</tr>
</tbody>
</table>
**Light-Operated Rotaxanes on Graphene**

**Introduction**
Rotaxanes as one species of mechanically interlocked molecular architecture are of a lot of concern today. Moreover, monolayer graphene which has remarkable electronic, optical and mechanical properties also attracts large amount of research interest. This research aims to combine the rotaxanes which are the macrocycle interlocked dumbbell shaped onto the monolayer graphene with a structure of two-dimensional hexagonal carbon lattice, and create an optical-controlled molecular machine. The new properties are tested and further applied into the areas such as molecular switches, molecular logic gates and molecular memories.

**Methodology and Results**
Schematic synthesis procedure for the photoinduced-switchable graphene-based rotaxane is as following.

**Scheme 1.** The synthesis of photoinduced-switchable [2]rotaxane functionalized graphene.

The hemi[2]rotaxane prepared by mixing one equiv of compound 6 and two equiv of the azo-CD ring in aqueous solution was evident by $^1$H NMR spectroscopy shown in Figure 1.

**Figure 1.** $^1$H NMR spectra of a) compound 6, b) after the addition of the azo-CD ring at 40 °C for 1 hour in the dark, and c) after irradiation by UV light at 365 nm for 3 hours.

Furthermore, UV-vis absorption spectrum of trans- and cis- form of graphene@rotaxane is shown below.

**Figure 3.** UV-vis absorption spectra of graphene@rotaxane in aqueous solution before any irradiation (red curve), followed by irradiation of 365 nm UV light for 10 mins (black curve), and last by irradiation of visible light for 15 mins (red curve). The inset slot shows the absorbance changes at 370 nm as a function of the cycle numbers of alternating UV and visible light irradiation.

**Conclusion**
A type of molecular machine consisting of reversible photo-switchable graphene@rotaxane has been designed, synthesized, and described. This molecular machine possesses of an α-cyclodextrane as a macromolecular switch, azobenzene as a photo-induced moiety, and monolayer graphene and 2,6-naphthalenedisulfonic acid disodium as the stoppers. More characterizations of this graphene@rotaxane will be done to determine its properties and further applied as molecular logic gates or molecular memories in the future work.

**Acknowledgement**
I would like to thank my supervisor Nanyang Assistant Professor Zhao Yanli and my mentor Dr Yan Hong for their guidance and ideas throughout this project. I would also like to extend my gratitude to all research staff and graduate students in Dr Zhao’s group who had helped me in one way or another.

**References**