

Heterocyclic Nanotube End-caps: Shape, Strain, and Function

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In this project we plan to obtain new chemical compounds, containing cap-shaped molecules. Because of their small size, we will call them “nanotube end-caps” or nanocaps for short (Figure 1). A molecule of this shape can evoke many associations with ordinary objects, and many people will agree that it actually resembles a hat. The analogy with headgear is actually productive if we recall the traditional Turkish hats, *kalpaks*, which were sewn from wedge-shaped panels, which tapered toward the top of the hat. Such a design is seen in V. V. Vereshchagin’s painting *Dervishes* (Figure 2).

We have recently found that nanocap molecules can indeed be “sewn” according to the above *kalpak* design. In chemistry, of course, we use chemical reactions to stitch the edges of the panels with chemical bonds (red in Figure 3). The chemical reaction has to do much more than just stitching, because unlike *kalpaks*, which were made of felt or sheepskin, our nanocaps are tailored from a very stiff material! This means, that the reaction has to put a lot of energy to bend the cap pattern into shape and hold it deftly during stitching. Our method does both things well and we think that it will allow us to sew “molecular *kalpaks*” of diverse shapes and sizes.

Nanocaps are just one type of cavity-containing molecules that can be shaped from small pieces of graphene, but chemists have only recently learned how to build these unusual structures (Figure 1). These molecules are highly interesting because they may be used in the future to build molecular electronic devices. We believe that our research can contribute to the understanding of their chemistry by providing not only new interesting molecules but also by inventing new ways to make them.

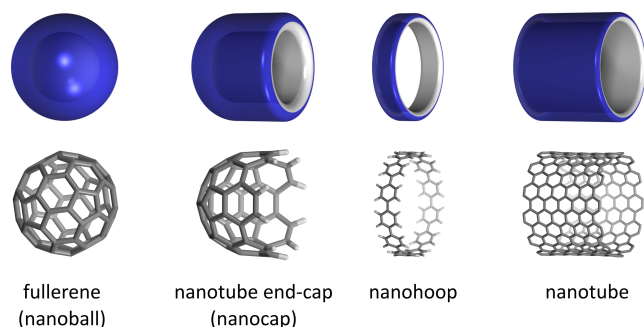


Figure 1. Carbon-rich molecules containing cavities.



Figure 2. *Dervishes in holiday costumes* (fragment). V. V. Vereshchagin, 1870.

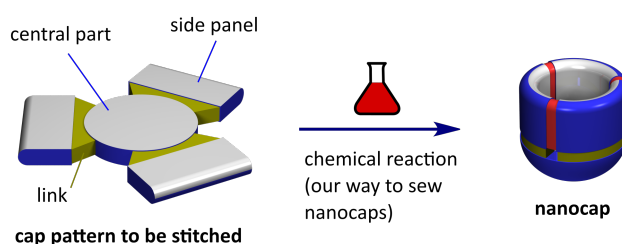


Figure 3. Our way to sew nanocaps.