

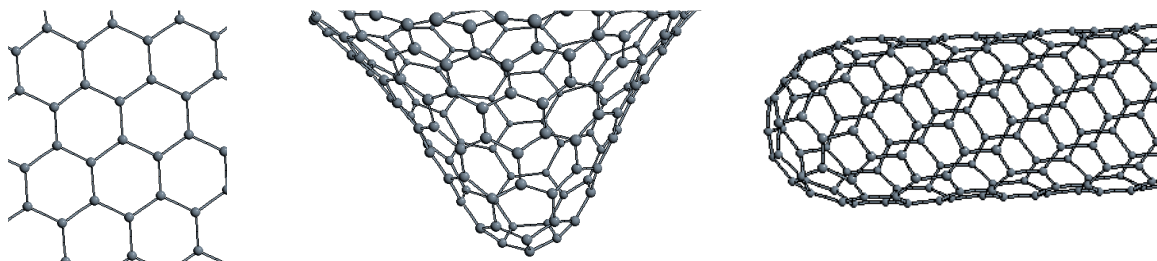
NANOCONES

A classification result in chemistry

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Nanococones are carbon networks conceptually situated in between graphite and the famous fullerene nanotubes. Graphite is a planar carbon network where each atom has three neighbours and the faces formed are all hexagons. Fullerene nanotubes are discussed in two forms: once the finite, closed version where except for hexagons you have 12 pentagons and once the one-side infinite version where 6 pentagons bend the molecule so that an infinite tube with constant diameter is formed. A nanococone lies in the middle of graphite and one-side infinite fullerene nanotubes: next to hexagons it has between 1 and 5 pentagons, so that neither the flat shape of graphite nor the constant diameter tube of the nanotubes can be formed. Recently the attention of the chemical world in nanococones has strongly increased. The figure below shows an overview of these types of carbon networks.



The structure of graphite is uniquely determined, but for nanotubes and nanococones an infinite variety of possibilities exist. There already exist fast algorithms to generate fullerene nanotubes (see [1]) that are e.g. used to detect energetically possible nanotubes. In this talk we describe a classification result and a generator for nanococones.

[1] G. Brinkmann, U. Von Nathusius and A.H.R. Palser, *A constructive enumeration of nanotube caps*, Discrete Applied Mathematics 116, 2002, pp. 55-71.