Graph-theoretical methods for the structural characterization of self-assembling nanoparticles

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In recent years there has been a growing interest in artificially engineered nanoshells, designed for instance to act as repetitive antigen displays for vaccines; such nanoparticles are made by repeated copies of a single polypeptidic unit, and their structural characterization is currently an open problem. In fact, they do not necessarily conform to the Caspar-Klug theory, which accounts for the arrangement of proteins in icosahedral spherical viruses, and there is no experimental technique allowing to resolve unambiguously their actual structure.
In this work I will show that graph-theoretical methods can provide important insights into the geometry of such nanoparticles.
I will study and classify the topology of the protein networks using tools from planar graph theory and tiling theory. Special attention will be devoted to symmetric particles, which can be fully described and classified.