THE MATHEMATICS OF SELF-ASSEMBLED PROTEIN NANOPARTICLES

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ABSTRACT. Self-assembly refers to the spontaneous organization of individual building blocks into higher order structures. It occurs in biological systems such as spherical viruses, which utilize icosahedral symmetry as a guiding principle for the assembly of coat proteins into a capsid shell. We characterize the de novo self-assembling protein nanoparticle (SAPN) system which was inspired by such viruses. Such artificially engineered nanoshells are made by repeated copies of a single protein or polypeptidic units. These pose new challenges for structure determination, since synthethic nanoparticles do not necessarily conform to the Caspar-Klug theory, which is the currently used template for the classification of viruses and, further, there is no experimental technique allowing to resolve unambiguously their actual structure. Here we discuss a mathematical framework for the classification and the prediction of the possible arrangements of the polypeptidic building blocks in self-assembling protein nanoparticles, studying the topology of the protein network using tools from graph theory and tiling theory. In particular, we present schematics that define the relative positions of all individual chains in the symmetric SAPN particles, and provide a guide of how this approach can be generalized to non-spherical morphologies, hence providing unprecedented insights into their geometries that can be exploited in future applications. (This work has been done in collaboration with N. Wahome, P. Ringler, S. A. Müller, M. Nieh, P. Burkhard, R. Twarock).

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