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Structural Complexity in Chiral Nanoassemblies and Biomimetic Composites

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Abstract: The structural complexity of composite biomaterials and biomineralized particles arises from the hierarchical ordering of inorganic building blocks over multiple scales. While empirical observations of complex nanoassemblies are abundant, physicochemical mechanisms leading to their geometrical complexity are still puzzling, especially for non-uniformly sized components. In the recent studies we developed graph theory (GT) for the description of nanoscale materials [1,2] and in this talk, I will describe how it can be applied to (a) chiral hierarchically organized particles (HOPs) with twisted spikes and other morphologies from polydisperse Au-Cys nanoplatelets [1] and (b) nanofibrous composites for batteries [2] and implantable electronics [3].

The complexity of Au-Cys HOPs is higher than biological counterparts or other complex particles as enumerated by graph theory (GT). Complexity Index (*CI*) and other GT parameters can be applied to a variety of different nanoscale materials to assess their structural organization. As the result of this analysis, we determined that intricate organization of HOPs emerges from competing chirality-dependent assembly restrictions that render assembly pathways primarily dependent on nanoparticle symmetry rather than size. These findings and HOPs phase diagrams open a pathway to a large family of colloids with complex architectures and unusual chiroptical and chemical properties.

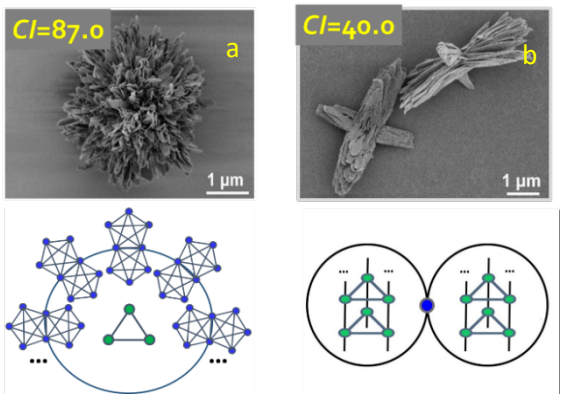

Fig. 1: HOPs self-assembled from chiral (**a**) and racemic (**b**) nanoparticles with corresponding graph theory models and complexity indexes (*CI*) [1].

Developed GT methods can also be applied to the design of complex biomimetic composites for energy and robotics applications [2] and implantable devices [3] establishing the relations between the functionalities and GT parameters of the biomimetic materials.

References

[1] W. Jiang, Z.-B. Qu, P. Kumar, D. Vecchio, Y. Wang, Y. Ma, J. H. Bahng, K.Bernardino, W. R. Gomes, F. M. Colombari, A. Lozada-Blanco, M. Veksler, E. Marino, A. Simon, C. Murray, S. Ricardo Muniz, A. F. de Moura, N. A. Kotov, Emergence of Complexity in Hierarchically Organized Chiral Particles, *Science*, **2020**, 368, 6491, 642-648.

[2] Wang, M.; Vecchio, D.; Wang, C.; Emre, A.; Xiao, X.; Jiang, Z.; Bogdan, P.; Huang, Y.; Kotov, N. A. Biomorphic Structural Batteries for Robotics. *Sci. Robot.* **2020,** 5 (45), eaba1912. https://doi.org/10.1126/scirobotics.aba1912.

[3] Huanan Zhang, Drew Vecchio, Ahmet Emre, Samantha Rahmani, Chong Cheng, Jian Zhu, Asish C. Misra, Joerg Lahann, Nicholas A. Kotov, Graph Theoretical Design of Biomimetic Aramid Nanofiber Nanocomposites as Insulation Coatings for Implantable Bioelectronics, **BioArxiv** doi: 2020, https://doi.org/10.1101/2020.12.28.424604