Emergence of Complexity in Chiral Nanoscale Assemblies and Graph Theory of Nanostructures

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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. Here we report the assembly of hierarchically organized particles (HOPs) with twisted spikes and other morphologies from polydisperse Au-Cys nanoplatelets [1]. 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. Developed GT methods can also be applied to the design of complex biomimetic composites for energy and robotics applications [2].

Prof. Nicholas A. Kotov is known foundational discoveries in biomimetic nanostructures and interface-based materials engineering that transcended multiple disciplines from chemical engineering to materials science, soft electronics, energy technologies, drug discovery, biomedical implants, and robotic devices. Examples of biomimetic nanostructures associated with his works include graphite oxide,- graphene- and clay-based layered biomimetic nanocomposites, chiral nanomaterials, and omni-dispersible colloids. He demonstrated that the ability to self-organize into complex structures is the unifying property of all nanostructures, inorganic, organic, or biological. Professor Kotov recreated the universal process by which complex biological structures are assembled and uncovered pathways that nature uses to create these materials. With this insight, he created versatile family of composite materials for various chemical engineering processes from gas separation to charge transport with extraordinary properties that had previously been deemed unattainable. Professor Kotov's research methodologies have seen widespread adoption by researchers and industries around the globe and is testament to the wide reach of his discoveries. His contribution to technology include ultrastrong nacre-mimetic nanocomposites, soft neuro-prosthetic implants, 3D tissue replicas for drug-testing, chiral biosensors, and cartilage-like electrolytes for batteries. Prof. Kotov is a founder of several start-up companies that commercialized bioinspired nanomaterials for biomedical, energy, military, automotive, and robotics technologies.

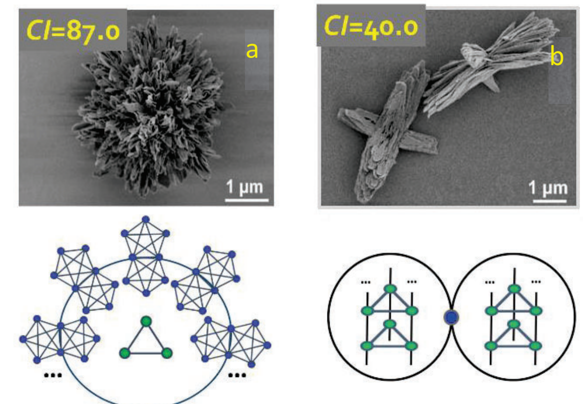

Fig. 1: HOPs self-assembled from chiral (**a**) and racemic (**b**) nanoparticles with corresponding graph theory models and complexity indexes (*CI*) [1].

References

[1] W. Jiang, N. A. Kotov et al, Emergence of Complexity in Hierarchically Organized Chiral Particles, *Science*, **2020**, 368, 6491, 642-648.

[2] M. Wang, N. A. Kotov et al, Biomorphic Structural Batteries for Robotics. *Sci. Robot.* **2020,** 5 (45), eaba1912. https://doi.org/10.1126/scirobotics.aba1912.