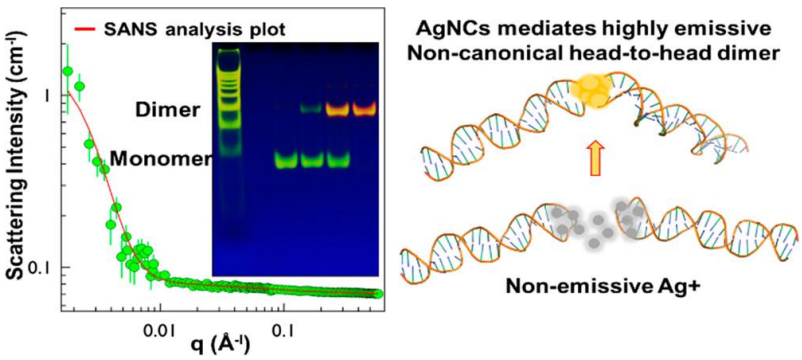
Noncanonical Head-to-Head Hairpin DNA Dimerization at Interfacial Binding Sites by Orange Emissive Silver Nanocluster

Pratik Shah [a,b]*
[a] Department of Science and Environment, Roskilde University, Denmark
[b] Department of Systems Biology, Yonsei University, South Korea
shah@ruc.dk

DNA has been employed as a versatile building block for assembly of nanomaterials due to its distinct programmability and predictability. One such fluorescent nanomaterial, DNA-stabilized silver nanoclusters (DNA-AgNCs), is an emerging tool for diverse applications ranging from biosensing, bioimaging and biocomputing. However, their optical properties, mechanism of formation, and aspects of their composition remain unexplored, making the rational design of nanocluster DNA templates challenging. DNA secondary structures, such as dimers and hairpins, are important for the synthesis of (DNA/AgNCs). However, the arrangement of AgNCs within a given DNA template and how the AgNCs influences the secondary structure of the DNA template are still unclear. Our current research in this direction has revealed an unnatural DNA secondary structure driven by the silver nanoclusters. Through detailed in-gel analysis, sugar backbone switching, inductively coupled plasma mass spectrometry, small-angle X-ray scattering, and small angle neutron scattering, we identified AgNCs mediated cytosine-Ag-cytosine bridging between two six-cytosine loop (6C-loop) hairpin DNA templates as a pre-requisite for the synthesis of orange emissive silver nanoclusters. Importantly, we did not detect formation of this unusual structure in the presence of Ag^+ ions. Moreover, we found that deoxyribose in the backbone of the 6C-loop at the third and fourth cytosines is crucial for the formation of the orange-emissive AgNCs and the head-to-head hairpin DNA structure.[1] This Noncanonical Head-to-Head Hairpin DNA Dimer is being investigated as the tool for early for disease diagnostics. Furthermore, the application of AgNCs in real-time monitoring of DNA structural dynamics in response to environmental stimuli is being explored.



[1] Pratik Shah, et.al. ***ACS Nano***., *2020, 14 (7),* 8697-8706.