Center for Dynamics and Control of Materials: *MRSEC Seminar*

Non-canonical DNA structures: Discoveries in perylene diimide self-assembly and DNA catalysis

Thursday, March 7th, 9:30 am-10:30 am

Texas Innovation Center, EER 2.518 – Same time and place as the IRG 1 meetings!

While the Watson-Crick double-helix structure of DNA is most widely known, other, non-canonical DNA structures are being investigated for their biological roles, utility in programable self-assembly, and potential to serve as catalysts. G-quadruplex DNA, a four-stranded DNA comprised of G-tetrads, is a non-canonical DNA structure that undergoes programable self-assembly and is also a potential drug target in cancer cells. Our work has identified small molecule ligands for G-quadruplex and revealed that certain perylenediimides (PDIs) are highly selective ligands for these structures. Our studies point to the well-known propensity of these compounds to undergo self-association as the origin of this selectivity. As part of this investigation, a remarkable case of LCST behavior in a PDI was discovered, and the structural basis for this property will be discussed. Recently, a non-canonical DNA structure related to G-quadruplex DNA, the three-stranded G-triplex has been described. Our recent work focuses on establishing the sequences and conditions that favor G-triplex formation, and investigations into the potential for G-triplex DNA to serve as catalyst. This has led to the identification of a robust G-triplex DNA structure that can serve as a peroxidase to enable chemiluminescence. The potential advantages of G-triplex-based DNA catalysis will be discussed.

Sean Kerwin is a professor and director of the Materials Science, Engineering, and Commercialization program at Texas State University. He earned his PhD in Chemistry at UC Berkeley, and began his academic career at UT Austin, moving to Texas State in 2015. His research interests span organic chemistry, biochemistry, medicinal chemistry, and materials science.

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