Diamondoid functionalized nanopores as biosensors

Jun.-Prof. Maria Fyta, Ganesh Sivaraman (C.9)

Solid state nanopores embedded with gold electrodes have been proposed to be strong candidates for the electrical read out of DNA. However, reduction in the noise in the electrical measurement is critical for an error free read out of DNA. A possible solution would be to use functionalized nanopores. In these, the specific interaction of a ”functionalizing molecule” with the DNA should increase the signal-to-noise ratio in the measurements. Recently, we have proposed amine- and thiol-doped diamondoids, as potential functionalizing molecules. Diamondoids are tiny hydrogen-terminated diamond clusters with a variety of doping and functionalization possibilities. These nanostructures can show strong quantum confinement effects and are potential candidates as nanoscale biosensors.

Along these lines, we first investigate the possibility of chemically modified diamondoids to detect biomolecules, such as DNA. Quantum mechanical calculations underline the specific interactions of diamondoids with DNA units and reveal the bonding characteristics and distinguishable electronic properties of diamondoid-DNA complexes. At a second step, we characterize the structure, electronic, and transport properties of Au(111) electrodes and diamondoid-functionalization on the Au(111) electrode surface. A small bias voltage is applied across the Au(111) electrodes in order to perform electronic transport measurements along a DNA placed between two diamondoid-functionalized surfaces. The aim is to use the tunneling current across the functionalized junction as a means for distinguishing between individual DNA nucleobases/mutations. We evaluate the tunneling current across the electrodes by inserting separately the 4 nucleotides, one mutant, and one epigenetic marker between the electrodes. In the end, we discuss the relevance of our results in view of biosensing applications and specifically nanopore sequencing of DNA.