DNA Methylation Detection Using 2D Material Nanopores

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Using molecular dynamics and electronic transport simulations, we show that graphene and Molybdenum-di sulphide (MoS_2) nanopores can be used to detect methylation in DNA. Methyl-CpG binding proteins are used to selectively label the methylated sites. The detection via ionic and transverse currents are carried out simultaneously and independently of each other. There is a strong correlation between the translocation of the methyl-CpG binding domain protein and detection via either of the sensing methods. The position of the methylation sites can be clearly recognized by the relative positions of the dips in the recorded ionic current blockade with an estimated error ranging from 0 to 16%. We also explore the limits of unique detection of two methyl-CpG binding domain proteins attached to methylated sites and the consequences of utilizing multi-layer nanopores for MBD protein detection. By defining the spatial resolution of the two-dimensional material nanopore device as the minimal distance between two methylation sites identified within a single measurement, it is 15 base pairs by ionic current recognition, but as low as 10 base pairs by transverse electronic conductance detection, indicating better resolution with this latter technique.

References

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