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Dual mechanisms of DNA sequencing based on tunnelling between nitrogen-doped carbon nanotube electrodes HAN SEUL KIM, YONG-HOON KIM, KAIST Graduate School of EEWS — The DNA sequencing approach based on the combination of nanopores and electron tunnelling has seen considerable advances in recent years, and particularly carbon nanomaterials have emerged as promising candidates to replace metal electrodes. Carrying out extensive first-principles calculations, we here show that two distinct DNA sequencing mechanisms can be achieved with different configurations of a single-type nitrogen-doped capped carbon nanotube (CNT) that has significantly enhanced transmission and chemical sensitivity over its pristine counterpart. With a small CNT-CNT gap size that induces face-on nucleobase configurations, we obtain a typical conductance ordering where the largest signal is induced from guanine due to its highest occupied molecular orbital energetic position higher than those of other bases. On the other hand, for a large CNT-CNT gap size that accommodates edge-on nucleobase configurations, we extract a completely different conductance ordering in which thymine results in the largest signal. We find that the latter novel nucleobase sensing mechanism originates from the nature of chemical connectivity between nitrogen-doped CNT caps and nucleobase functional groups that include the thymine methyl group. This work thus demonstrates the feasibility of a tunnelling-based dual-mode approach toward whole genome sequencing applications, detection of DNA base modifications, and single-molecule sensing in general.

Yong-Hoon Kim
KAIST Graduate School of EEWS

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