Single-Molecule Probing By Rectification in a Nanogap

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Abstract. Here in this talk, we propose the simultaneous measurement of rectification and amplitude of tunneling current during electrical probing of a molecule in a nanogap for efficient single-molecule detection. Also, we suggest the application of nitrogen-terminated graphene or CNT nanogaps due to their inherent outstanding features. With DFT and Non-Equilibrium Green's Function formalism, we show that tunneling current through various molecules, including ssDNA, TATP, or small organics placed in those nanogaps, exhibits unique rectification behavior under square pulses of alternating bias. The rectification arises by on-off switching of electronic transport through the molecular HOMO or LUMO levels, sustained by partial charging of the probed molecule, generated by asymmetric hybridization of that level with Bloch states from one of the electrodes. An effect that mimics local gating, i. e. an interaction between the molecule and the nitrogen-induced dipole moment located at the N-C interface of the electrode ends, strongly influences the rectification. The simultaneous measurement of rectification and amplitude of tunneling current could be applied to gas-phase single-molecule detection, as shown in the example case of the TATP. The TATP (triacetone triperoxide) is a volatile, potent, and hard-to-detect explosive made from commonly available chemicals, a terrorist weapon of choice in the last two decades. The rectification could also be applied in the liquid phase, offering the possibility of high-throughput and precise DNA sequencing. We found that the environment (neighboring nucleotides, water molecules, and counterions) does not mask ssDNA rectification while ssDNA traverses the nanogap.

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