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Supplementary Information

Sensing Single Molecules with Carbon-Boron-Nitride Nanotubes

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Fig S1: Local Density of States for the energy range $E_F - 0.01 \rightarrow E_F + 0.01$ for the 1BN junction



Fig S2: Transport curves for junctions a-e of Figure 1, which compare with an Ideal CNT (line in red).



Fig S3: Conductance of the junction as a function of electrode separation.



Fig S4: Example of the benzene-doped junction.



Fig S5: Plot of the logarithm of the transport of the benzene-doped junction, $log_{10}(T(E))$, for different junction sizes (1BN-5BN). The darker lines represent the corresponding transport of the clean junction – also shown in figure 1. For each junction, the benzene rings were placed at several locations.



Fig S6: Plot of the logarithm of the transport of the pyridine-capped oligoyne-doped junction, $log_{10}(T(E))$, for 1BN to 5BN. The darker lines represent the corresponding transport of the clean junction – also shown in Fig 1. For each junction, the pyridine-capped oligoyne was placed at several locations.



Fig S7: The probability distribution $P_X(\alpha)$ of the set $\{\alpha_{X,m}(E)\}$ for (a) 1BN junction with benzene (blue), 1BN junction with PY (green), 1BN junction with SH (red) and ideal CNT with benzene (turquoise). (b) 2BN junction with benzene (blue), 2BN junction with PY (green), 2BN junction with SH (red) and ideal CNT with benzene (turquoise). (c) 3BN junction with benzene (blue), 3BN junction with PY (green), 3BN junction with SH (red) and ideal CNT with benzene (blue), 4BN junction with benzene (blue), 4BN junction with benzene (blue), 4BN junction with benzene (blue), 5BN junction with PY (green), 5BN junction with PY (green), 5BN junction with benzene (turquoise).





Fig S8: Left figure shows examples configurations of the 1BN junctions with benzene molecule, the benzene molecule shifted in a series of equally-spaced steps from the left side to right side. Right figure shows examples of configurations of the 1BN junction with a pyridine molecule.