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**Supplementary Information** 



Figure S1: Molecular energy levels for isolated nucleobase (A, T, C and G) of DNA. Fermi level is set at 0 eV.



**Figure S2:** Molecular electron density of states (DOS) for isolated nucleobase (A, T, C and G) of DNA. Fermi level is set at 0 eV.



Figure S3. A schematic of the STM like setup for Guanine +  $MoS_2$ .



Figure S4. A two terminal configuration of the transport model for G +MoS<sub>2</sub> conjugate system.



Figure S5. Transmission coefficients as a function of energy for pristine and nucleobase adsorbed MoS<sub>2</sub>.