

## Tuning molecular fluctuation to boost the conductance in DNA based molecular wire : Supporting Information

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### Section I: Effect of Na<sup>+</sup> ions on the frontier molecular orbitals (FMO)

To check the effect of the Na<sup>+</sup> ions on the frontier molecular orbitals (FMO), we now calculated the FMOs of a Guanine dimer (see Figure S1 below), chosen from the G4-Quad structure. We performed calculation with Na<sup>+</sup> ions and without Na<sup>+</sup> ions taken into account and found that the FMOs remains unaltered.

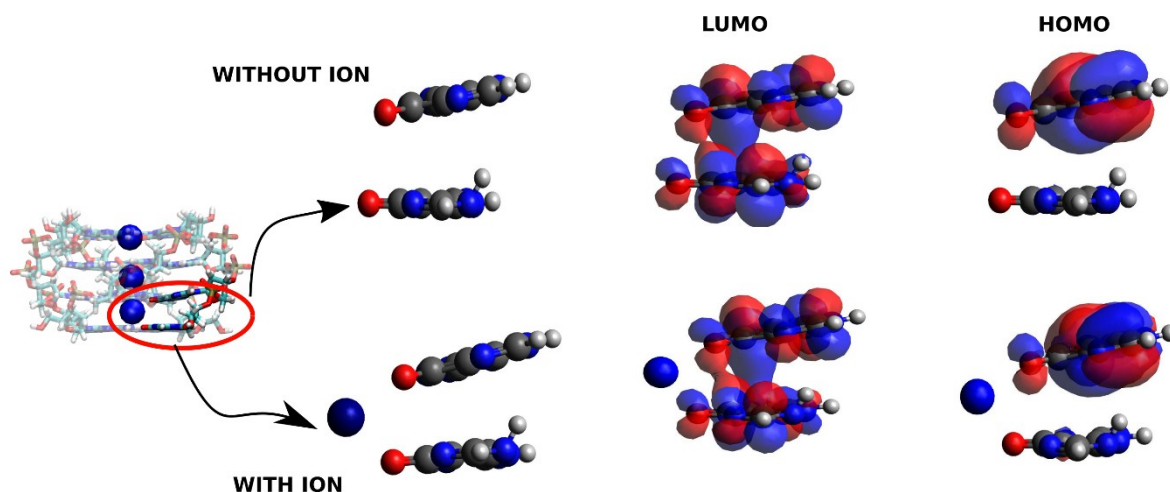


Fig: S1: LUMO and HOMO of a Guanine dimer in a G4-Quad Structure. LUMO and HOMO remain unaltered with the inclusion of Na<sup>+</sup> ions in the DFT calculation.