

SUPPORTING INFORMATION

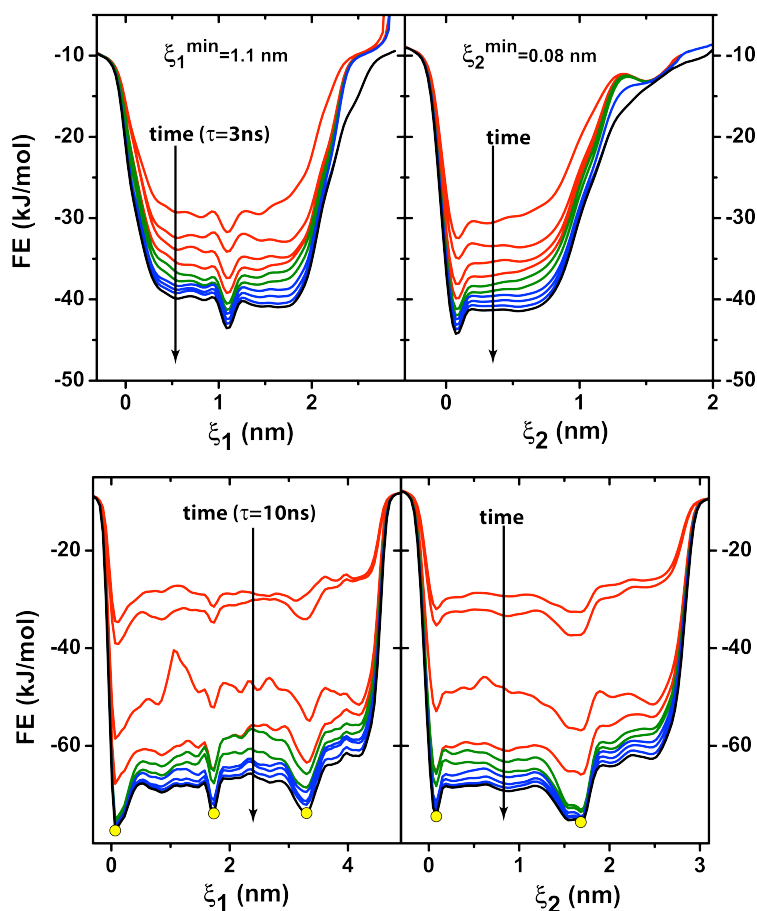


Figure S11. Convergence profiles of the metadynamics order parameters: *top*) A@hydrophobic (16,0) SWCNT and *bottom*) T@electrically charged (23,0) SWCNT. Each line corresponds to τ ns integration time of eqn.6 performed for each order parameter, $FE(\zeta) = -\frac{1}{\tau} \int_{t_{tot}-\tau}^{t_{tot}} V(\zeta, t)$, and the yellow dots are the three relative free energy minima. Note that the overall $FE(\xi_1)$ and $FE(\xi_2)$ lines, depicted in black, overlap the final τ ns timewindow. It becomes clear that the free-energy profiles are essentially converged to the corresponding minima; the energetic landscapes recorded in Fig. 2 and Fig.4 are accurate representations of the thermodynamical free-energy changes associated with the confinement process.

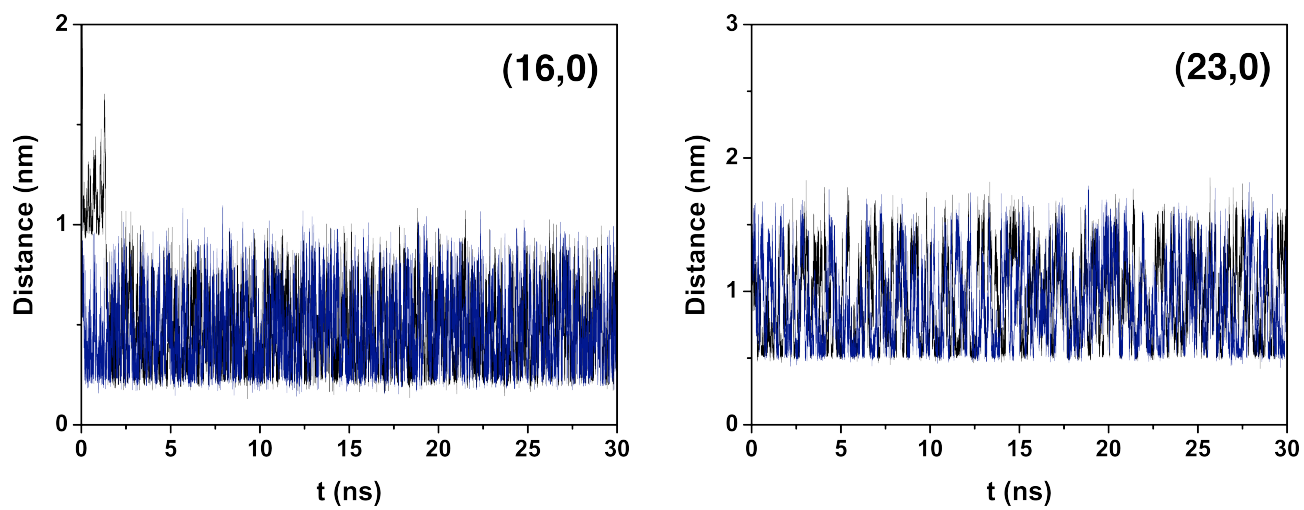


Figure SI2. Center of mass distance between nucleobase and hydrophobic SWCNTs observed in the unbiased calculations: *black*) adenine, *blue*) thymine.

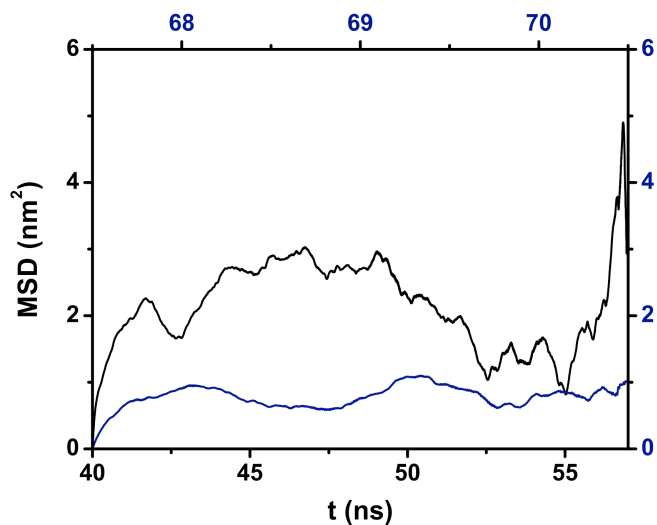


Figure SI3. Mean squared displacement of a nucleobase c.o.m. confined in a (23,0) electrically charged carbon nanotube, $MSD = \langle \|\mathbf{r}(t) - \mathbf{r}(0)\|^2 \rangle$, where $\mathbf{r}(t)$ is the NB positional vector at time t , and the triangular brackets denote an ensemble average: *black*) adenine and *blue*) thymine.

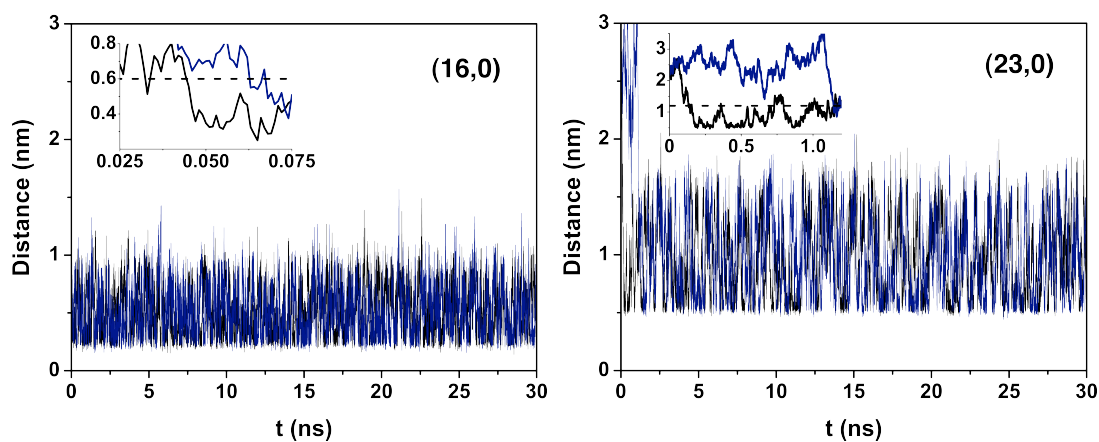


Figure SI4. Center of mass distance between nucleobase and hydrophobic SWCNTs: *black*) adenine, *blue*) thymine. The dashed line in the inset magnifications indicates an exact distance between nucleobase and SWCNT center of 0.6 nm (16,0) and 1.2 nm (23,0).

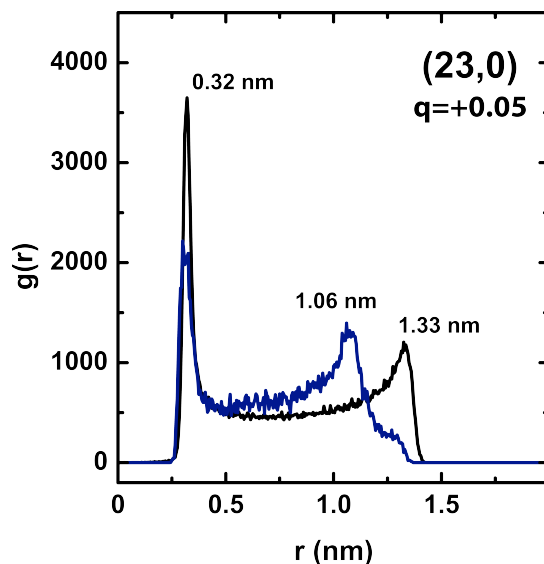


Figure SI5. Radial distribution functions between the nucleobase surface and the electrically charged (23,0) nanotube, calculated during the occurrence of a confinement event: *black*) adenine, *blue*) thymine.

Animations SI1-SI2. The first 1 ns of calculations is exemplified here for adenine in contact with the hydrophobic (23,0) nanotube; each s in the animations corresponds to 3.03×10^{-2} ns of real (simulation) time. H_2O molecules are represented by a red sphere corresponding to their O atom and the (23,0) SWCNT is depicted by a grey mesh. The annular concentric layers surrounding the solid walls, devoid of particles, are a direct consequence of the graphitic C atoms collision diameter. Notice the almost perfect parallel alignment between the NB and the inner walls, always maintained throughout confinement.