Supplementary Material (ESI) for Nanoscale

A multiscale simulation study of carbon nanotube interactions with designed amphiphilic peptide helices

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Supplementary Methods

Details of the OPLS simulation setup

All simulations performed with the OPLS force field[1, 2] used the GROMACS 3.3 software package.[3, 4] The simulations were performed at constant temperature (300K or 323 K), pressure (1 bar) and number of particles. All simulation parameters were as described for the GROMOS53A6 force field simulations.

Supplementary Figures

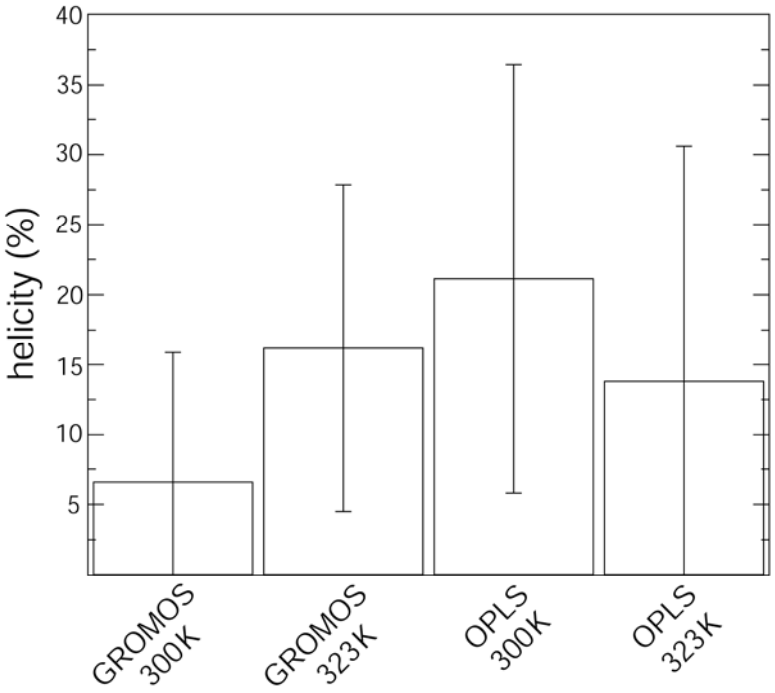
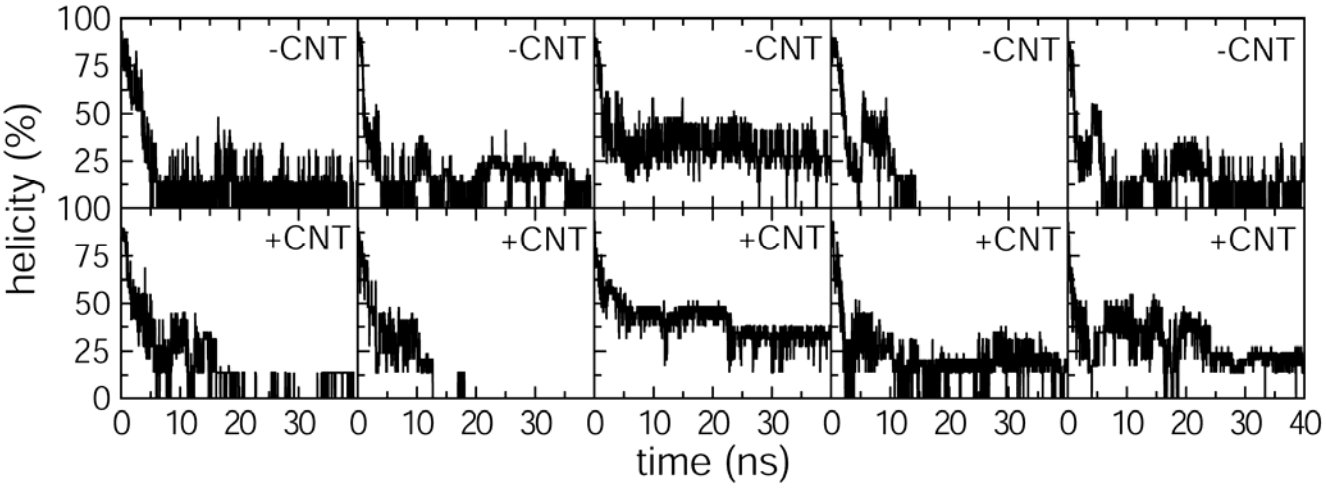


Figure S1. AT nano-1 α-helicity. An unrestrained nano-1 peptide was simulated in water with counter ions present. The initial simulation box dimensions were set to 70 x 70 x 70 $Å^3$. Simulations of nano-1 were performed with the GROMOS53A6[5] and OPLS[1, 2] force fields at 300 K and 323 K. Data was averaged between 30 to 40 ns over 3 simulations. Peptide α-helicity was evaluated using DSSP.[6]



b.

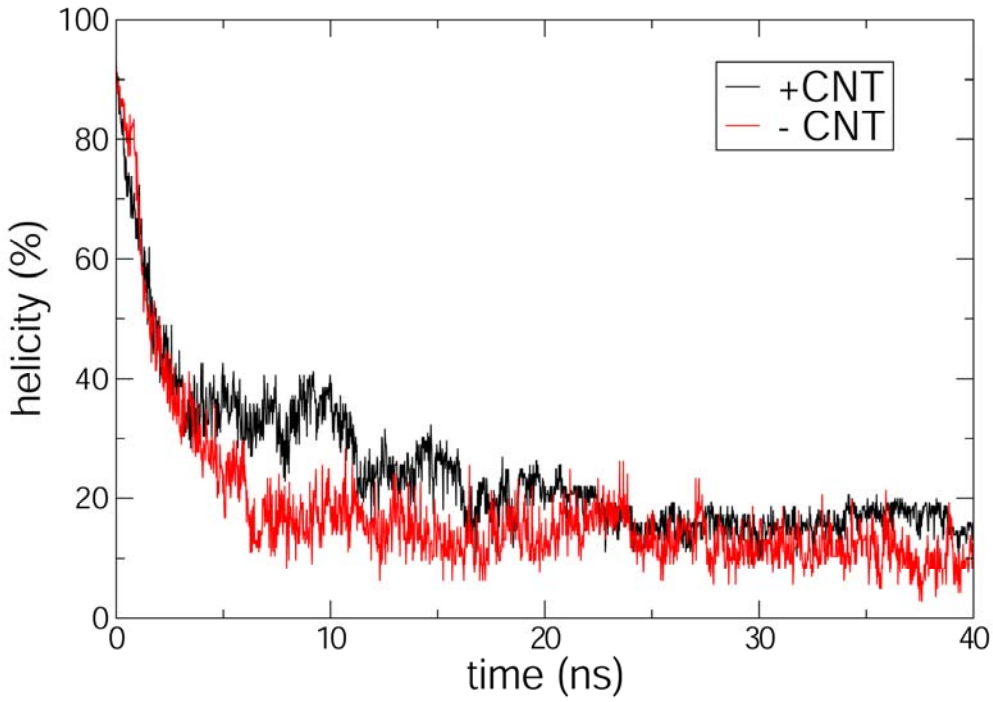


Figure S2. (a) AT nano-1 α-helicity as a function of time for a single peptide simulated in water (-CNT), and for a single peptide adsorbed onto a CNT surface (+CNT) that is simulated in water. The initial simulation box dimensions were set to 70 x 70 x 70 $Å^3$. (b) Average nano-1 α-helicity as a function of time. The average was determined over all 5 profiles calculated in the absence and presence of a CNT, as shown in part a.

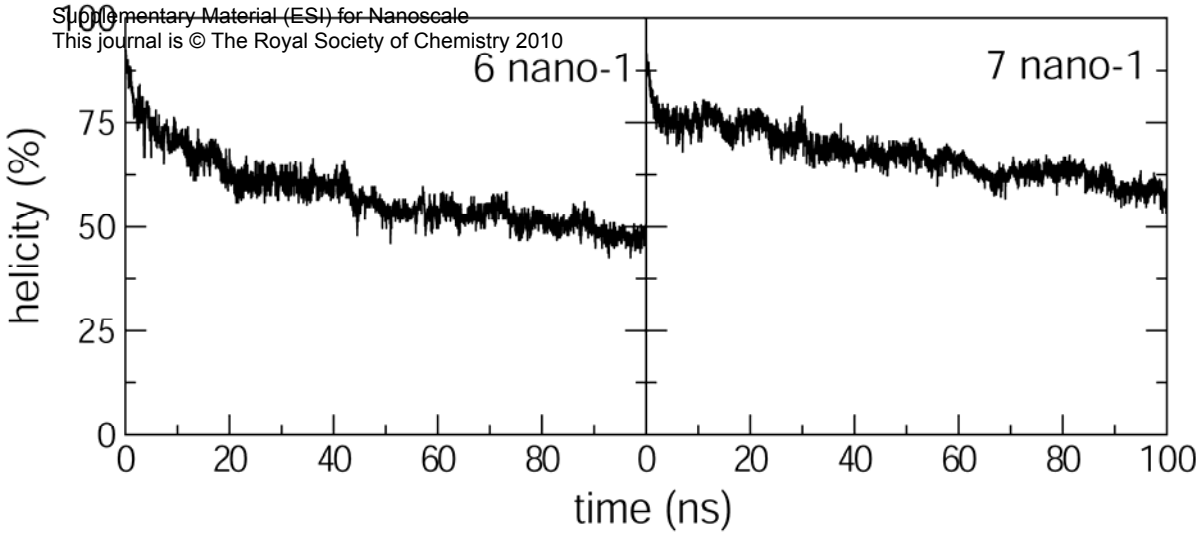


Figure S3. AT nano-1 α-helicity as a function of time for multiple peptides adsorbed onto a CNT surface.

References

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