Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information: The Effects of Water Molecules on the Electronic and Structural Properties of Peptide Nanotubes.

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Structure

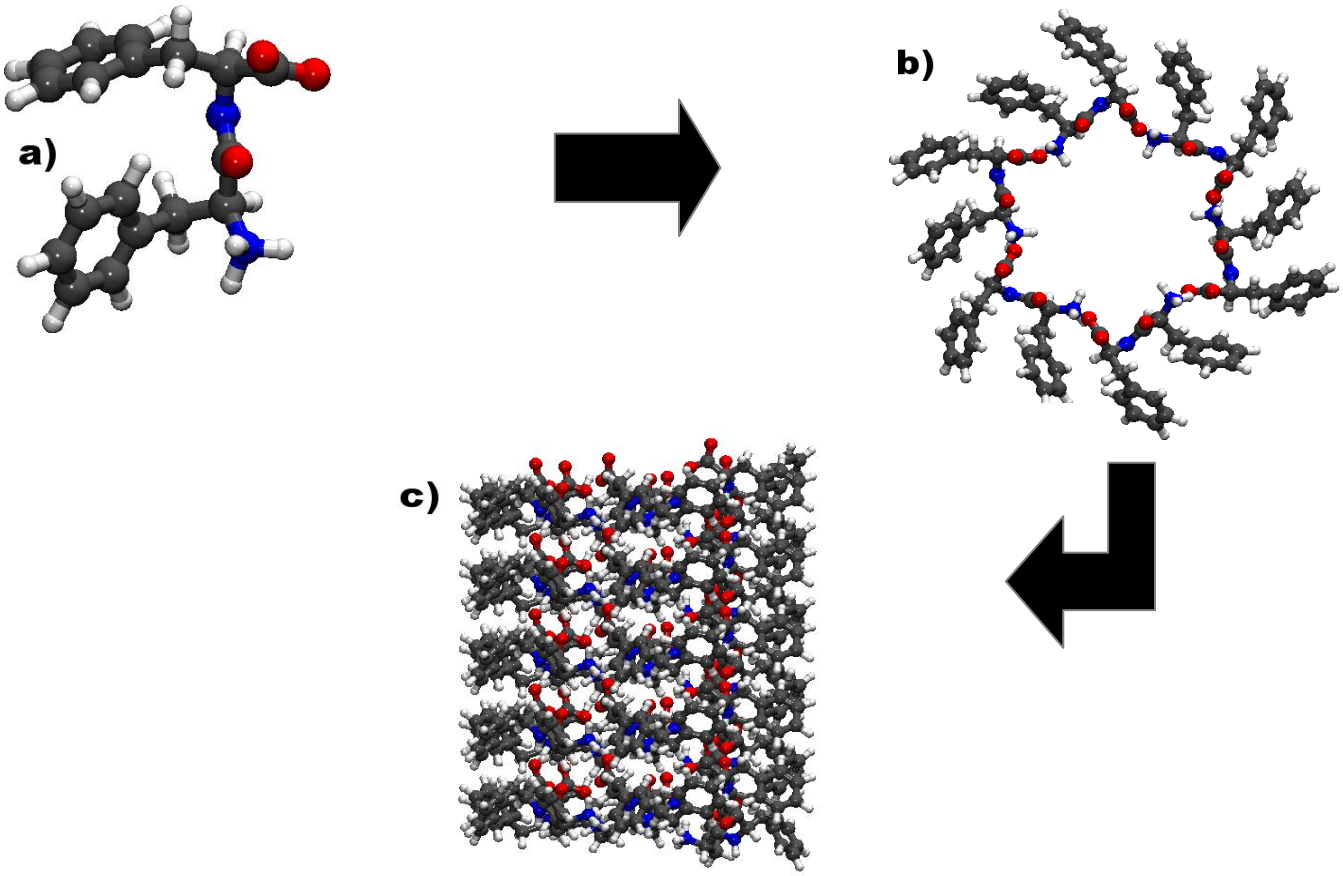

Figure S1- a) FF residue molecule, b) hexamer formation (unit cell structure used in this work) and the further vertical packing of hexamers forming a FF NT.

Methodology

The relaxation of lattice vector along the NT (axis c) and the atomic coordinates within the unit cell was performed at the SCC-DFTB-D method for both

systems. The lattice parameters are a = b = 44.00 Å and c = 5.51 Å for both anhydrous and hydrous systems. The simulation procedure occurred as follows: After relaxing the atomic coordinates of the anhydrous NT by means of the conjugate gradient method we confined 15, 17 and 24 water molecules in the hydrophilic channel of the NT. These numbers of water molecules were chosen according to the available average observations of Kim et al.,1 Görbitz[2] and Wang *et al.*[3]. The position of each confined water molecule was first optimized using the Packmol package [4,5]. Afterwards, the composite systems were relaxed also with the conjugate gradient method using a convergence criterion of 1.0×10^{-3} eV / Å.

References

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