Supporting Information For

Planar Boronic Graphene and Nitrogenized Graphene Heterostructure for Protein Stretch and Confinement

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Context:

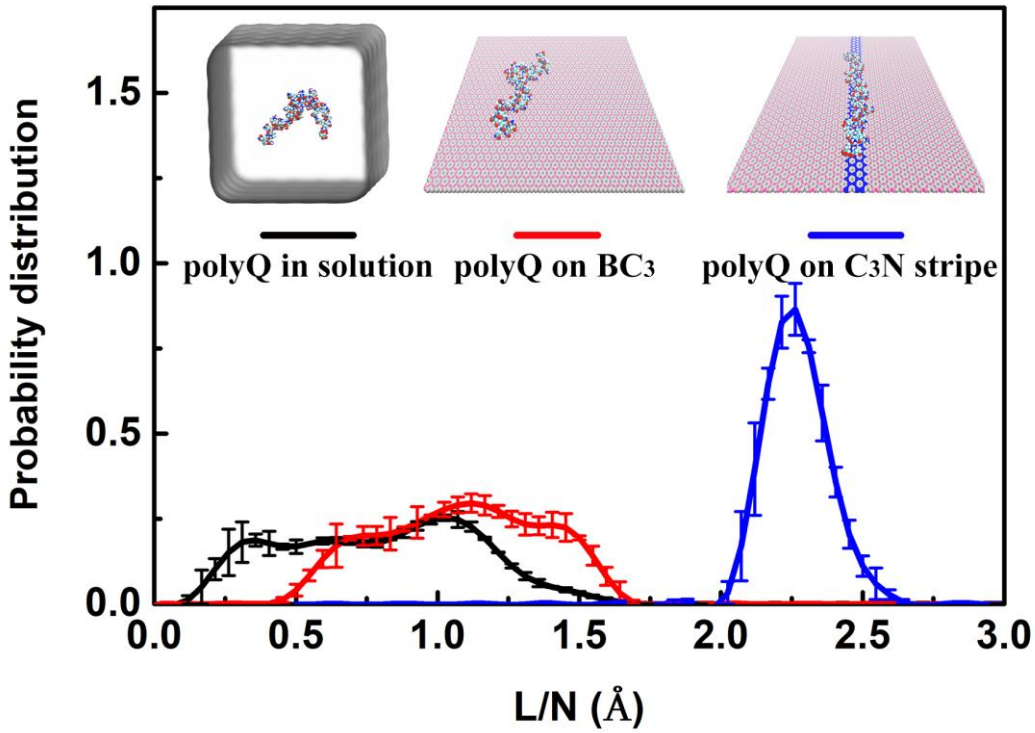

Fig. S1 Probability distribution of end-to-end distances for polyQ in solution (black line), on BC_3 (red line), and the C_3N stripe (blue line).

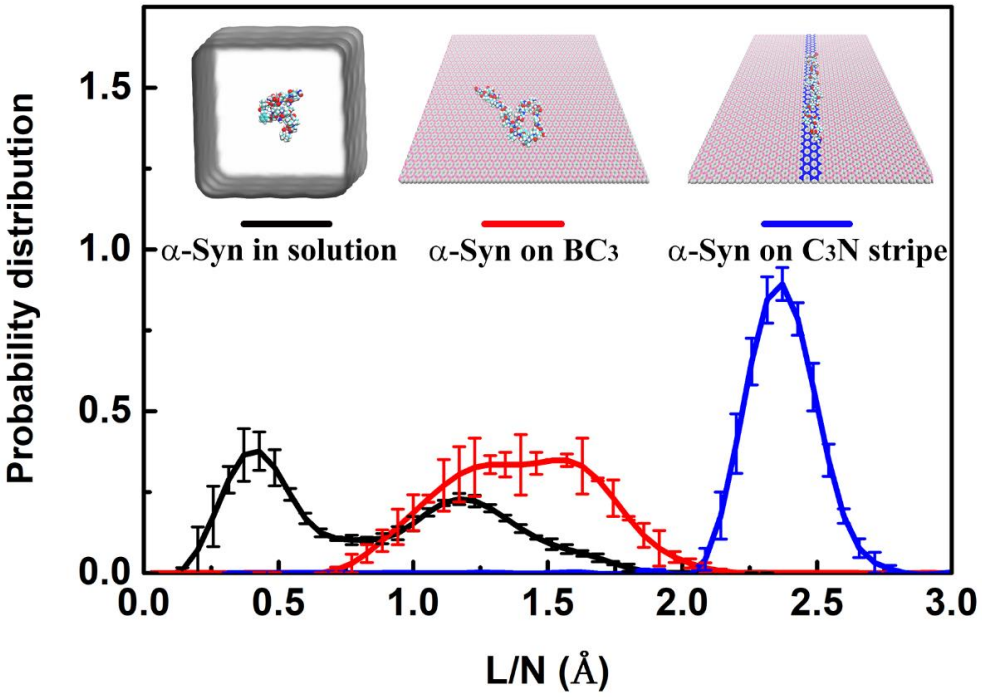

Fig. S2 Probability distribution of end-to-end distances for α-Syn in solution (black line), on BC_3 (red line), and the C_3N stripe (blue line).

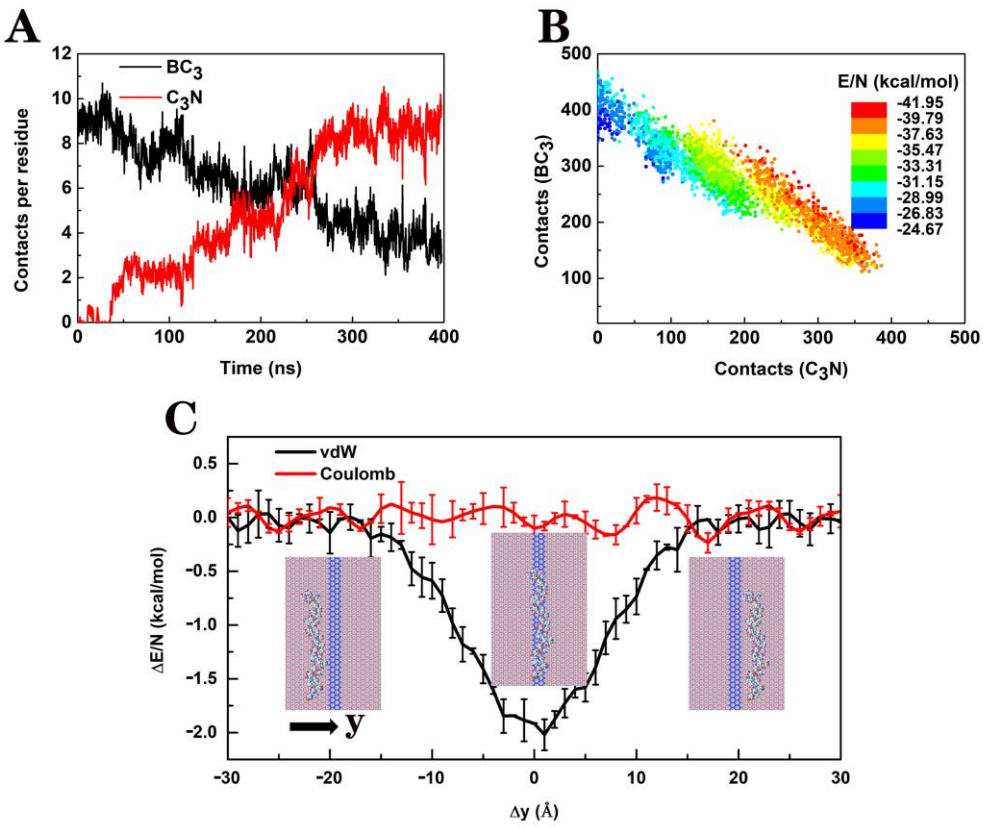

Fig. S3 (A) Number of atoms in $BC_3/C_3N/BC_3$ that are within 4.0 Å of the polyQ peptide throughout the simulation. (B) A scatter plot of the number of atoms in $BC_3/C_3N/BC_3$ in contact with polyQ. The color represents the average interaction energy per residue between polyQ and $BC_3/C_3N/BC_3$. (C) A smoothed curve of van der Waals (black line) and Coulomb (red line) interaction energy between polyQ and $BC_3/C_3N/BC_3$, when the elongated polyQ peptide moved across the C_3N stripe in the y-direction.

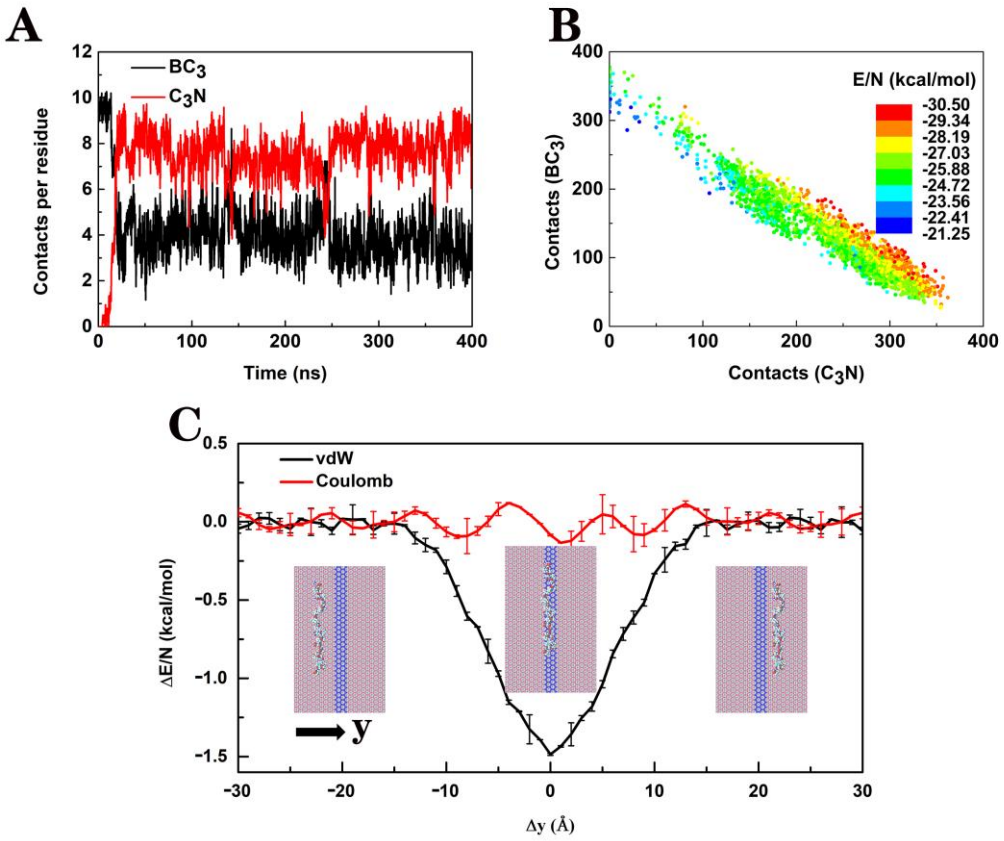

Fig. S4 (A) Number of atoms in $BC_3/C_3N/BC_3$ that are within 4.0 Å of the α-Syn peptide throughout the simulation. (B) A scatter plot of the number of atoms in $BC_3/C_3N/BC_3$ in contact with α-Syn. The color represents the average interaction energy per residue between α-Syn and $BC_3/C_3N/BC_3$. (C) A smoothed curve of van der Waals (black line) and Coulomb (red line) interaction energy between α-Syn and $BC_3/C_3N/BC_3$, when the elongated α-Syn peptide moved across the C_3N stripe in the y-direction.

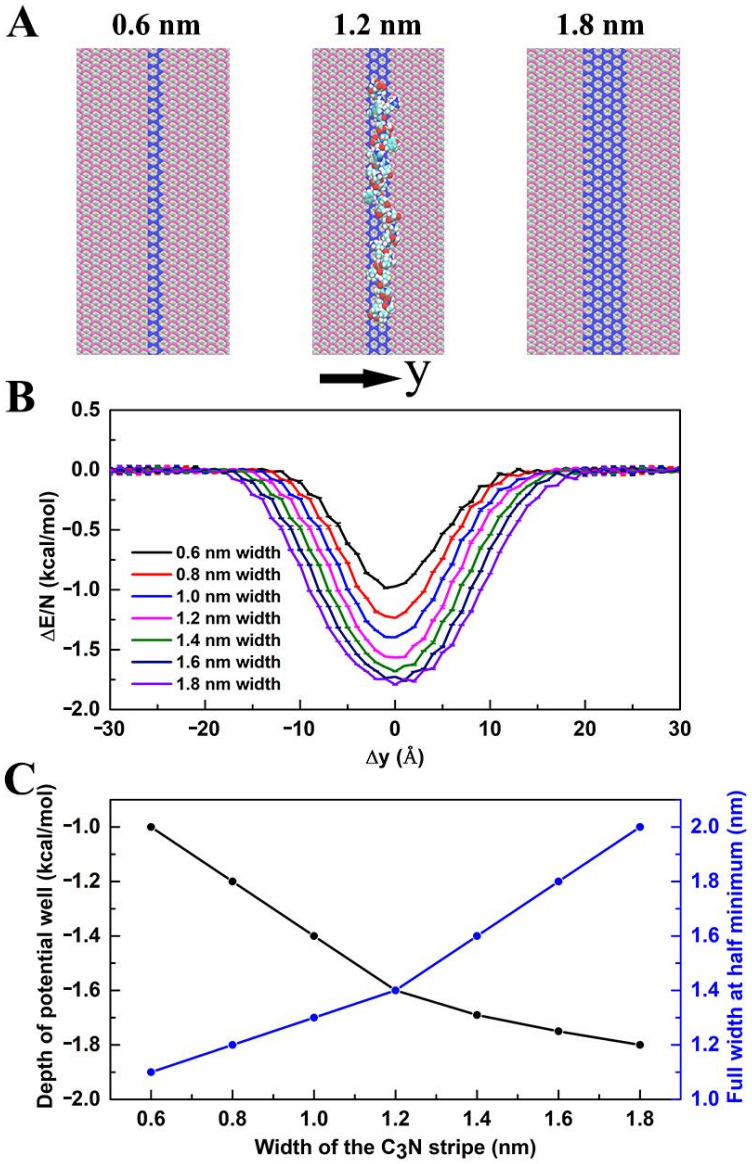

Fig. S5 Influence of the C_3N stripe width on the potential well for the straightened Aβ peptide. (A) Representative illustrations of C_3N stripes with widths of 0.6 nm, 1.2 nm, and 1.8 nm, respectively. The Aβ peptide elongated on the 1.2-nm-width C_3N stripe was used for the energy scan of each potential well. (B) Smoothed curves of van der Waals interaction energies between Aβ and $BC_3/C_3N/BC_3$, when the elongated Aβ peptide moved across each C_3N stripe with different widths in the y-direction. (C) The "potential-depth" (black line) and the "potential-width" at half-minimum of each well as a function of the C_3N stripe width.