

## Supporting Information For

### Planar Graphene/h-BN/Graphene Heterostructure for Protein Stretch and Confinement

Zhi He<sup>1,2</sup>, and Ruhong Zhou<sup>1,3\*</sup>

<sup>1</sup>Institute of Quantitative Biology, Zhejiang University, Hangzhou 310027, China

<sup>2</sup>College of Optical Science and Engineering, Zhejiang University, Hangzhou 310027, China

<sup>3</sup>Department of Chemistry, Columbia University, New York, NY 10027, USA

#### Context:

Movie S1. A representative movie showing the dynamical process of A $\beta$ <sub>1-42</sub> adsorption onto the graphene surface, peptide transfer at the boundary of graphene and h-BN, and the final peptide confinement/stretching on the h-BN stripe.

Fig. S1. Representative snapshots of the diffusion process of A $\beta$ <sub>1-42</sub> from the graphene surface to the h-BN stripe.

Fig. S2. Analysis of the polyQ<sub>42</sub> stretching process on the Graphene/Hexagonal Boron Nitride/Graphene (GRA/BN/GRA) heterostructure.

Fig. S3. Analysis of the  $\alpha$ -Syn<sub>61-95</sub> stretching process on GRA/BN/GRA.



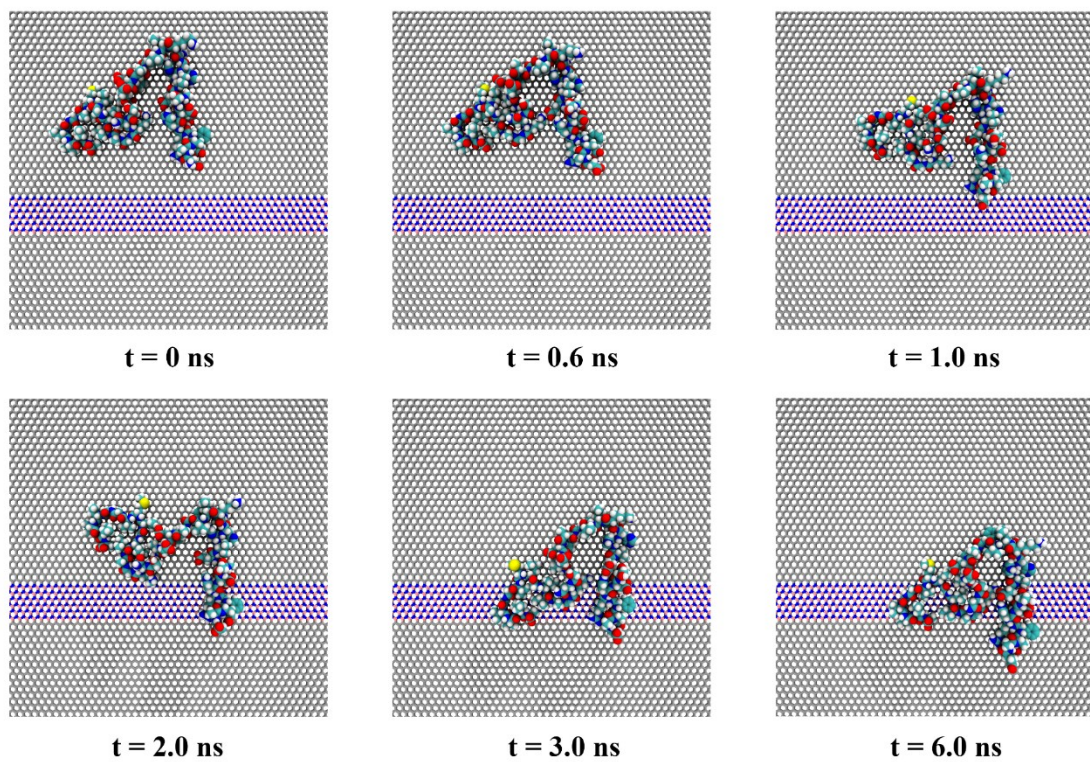


Fig. S1. Representative snapshots of the diffusion process of  $A\beta_{1-42}$  from the graphene surface to the h-BN stripe.



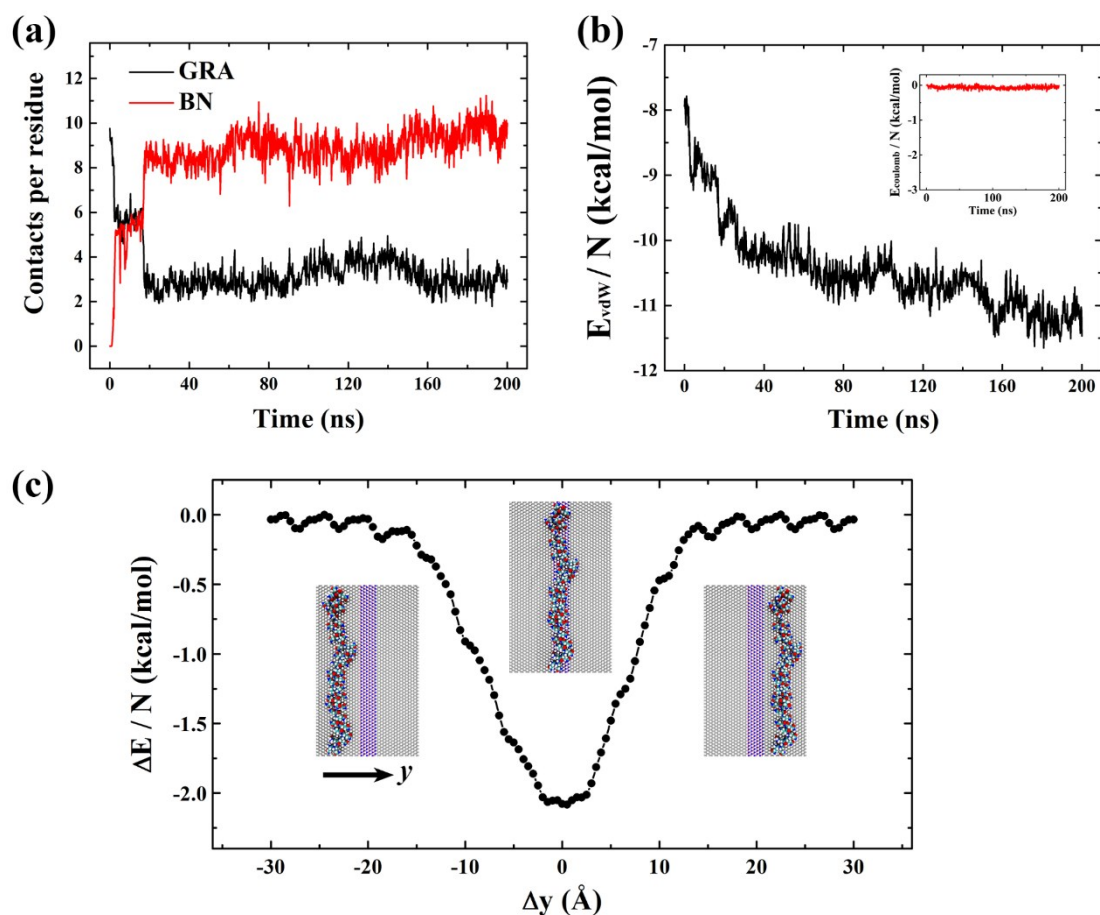


Fig. S2 (a) Number of atoms in GRA/BN/GRA that are within 4.0 Å of the polyQ peptide throughout the simulation. (b) The van der Waals interaction energy per residue between polyQ and GRA/BN/GRA. Inset: Coulomb interaction energy per residue between polyQ and GRA/BN/GRA. (c) Interaction energy between polyQ and GRA/BN/GRA when the elongated polyQ peptide moves in the y direction across the h-BN stripe.



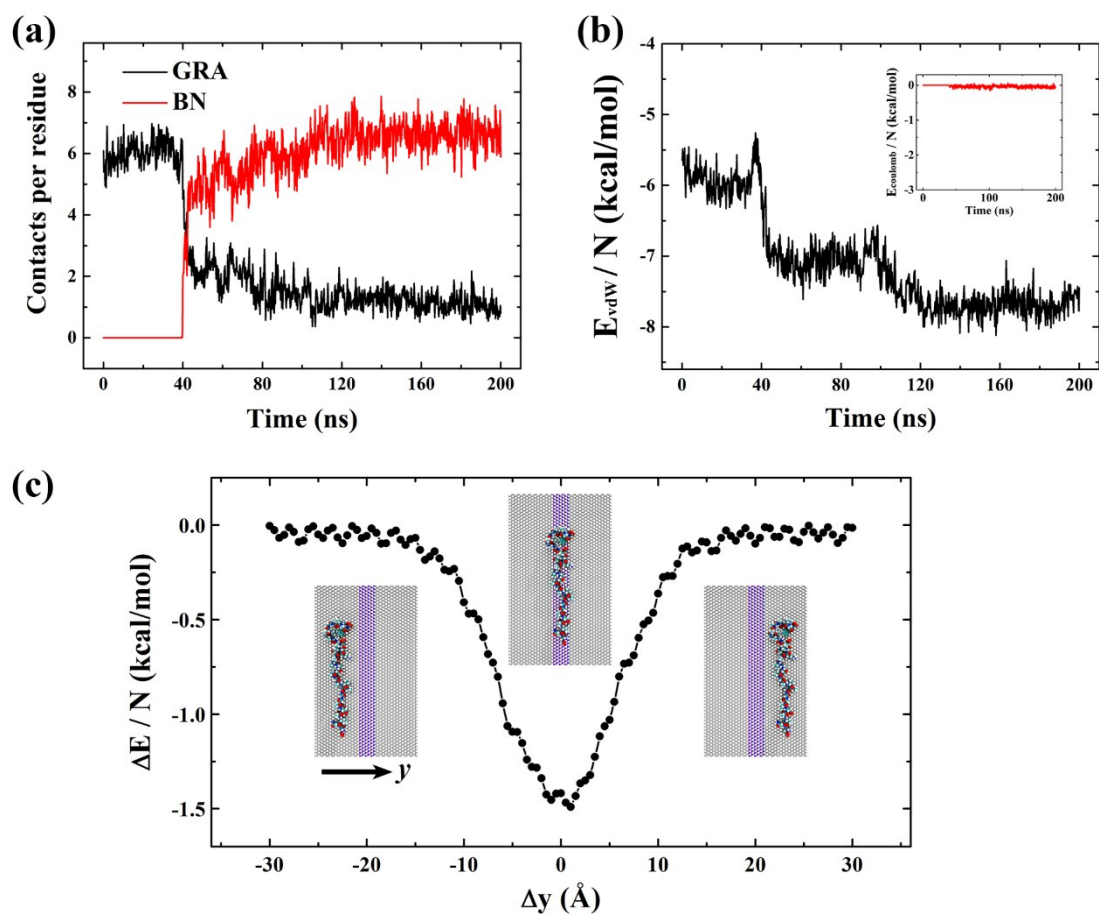


Fig. S3 (a) Number of atoms in GRA/BN/GRA that are within 4.0 Å of the  $\alpha$ -Syn peptide during the simulation. (b) The van der Waals interaction energy per residue between  $\alpha$ -Syn and GRA/BN/GRA. Inset: Coulomb interaction energy per residue between  $\alpha$ -Syn and GRA/BN/GRA. (c) Interaction energy between  $\alpha$ -Syn and GRA/BN/GRA when the elongated  $\alpha$ -Syn peptide moves in the y direction across the h-BN stripe.