

Supporting Information

Wrinkled Nanosurface Causes Accelerated Protein Unfolding Revealing Its Critical Role in Nanotoxicity

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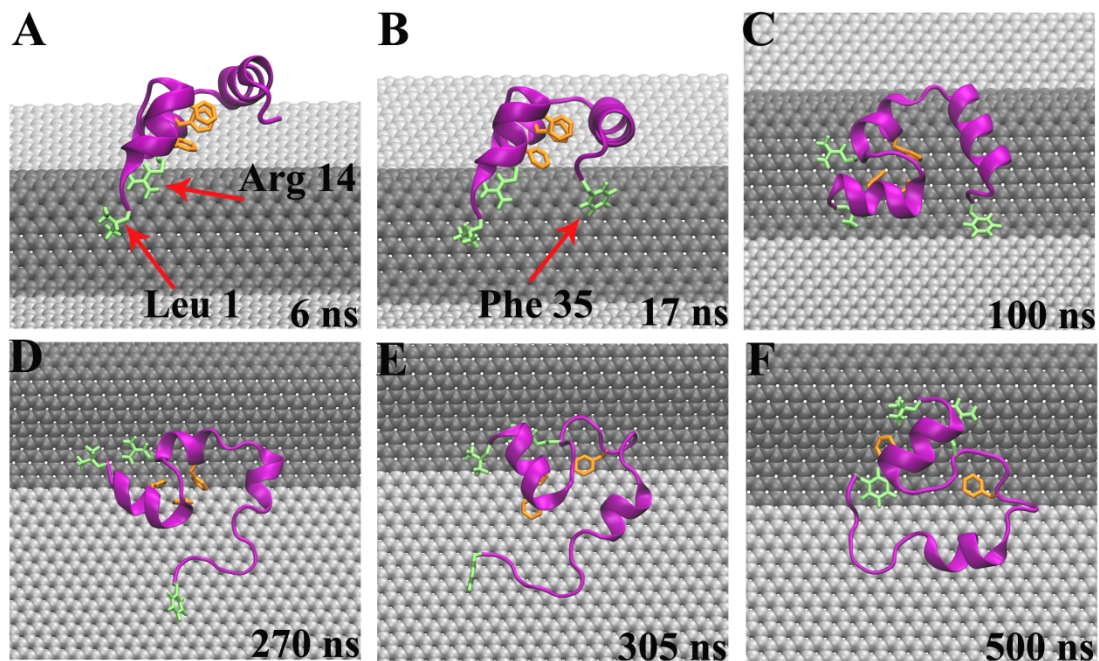


Figure S1. Structural evolutions of HP35 on W-Gra surface in traj-2. The hydrophobic core of HP35 is shown as orange sticks. The residues Leu 1, Arg 14 and Phe 35 that play important role in the unfolding process are shown as lime sticks.

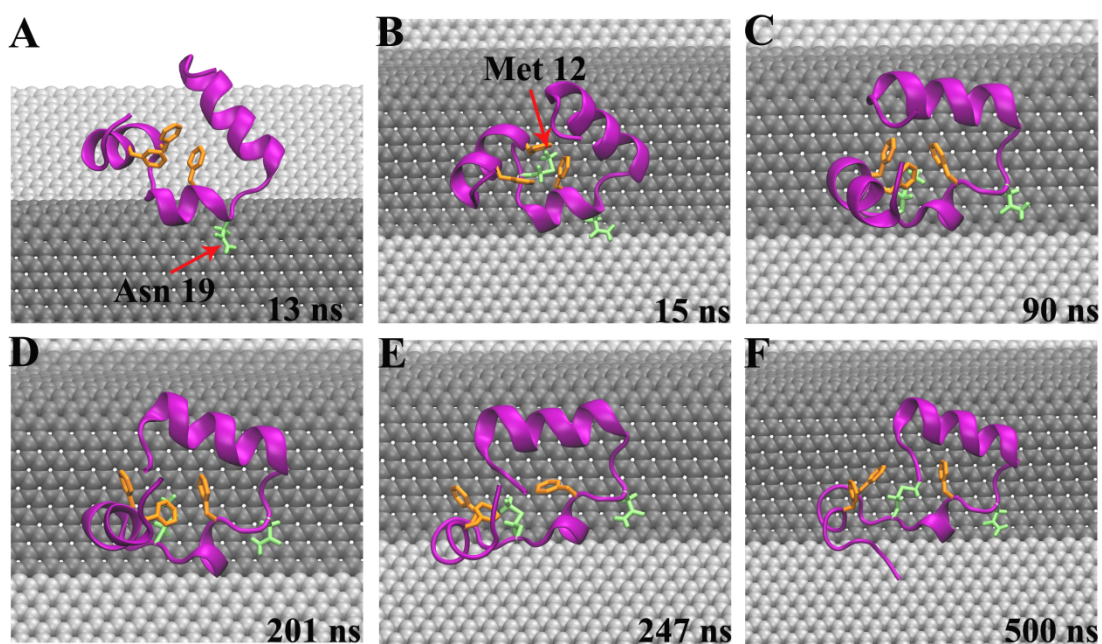


Figure S2. Structural evolutions of HP35 on W-Gra surface in traj-3. The hydrophobic core of HP35 is shown as orange sticks. The residues Met 12 and Asn 19 that play important role in the unfolding process are shown as lime sticks.

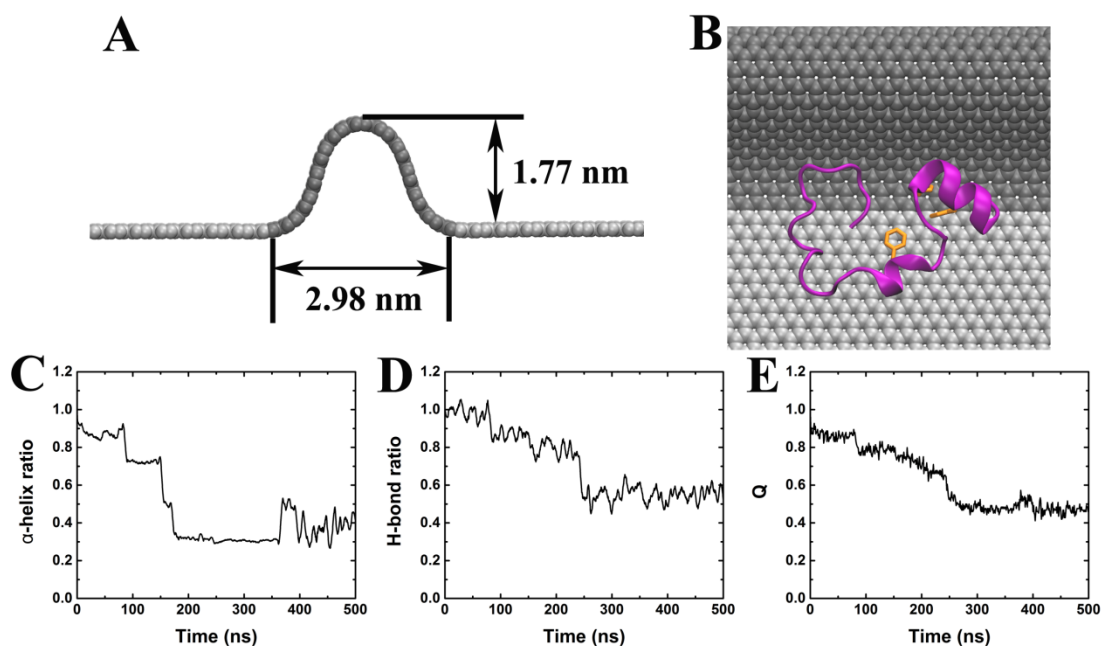


Figure S3. The simulation of the interactions between HP35 and graphene with a larger-sized wrinkle (abbreviated as LW-Gra). (A) The structure of the LW-Gra nanosheet. The carbon atoms in the wrinkled area are shown as dark gray spheres while the others are shown as light gray spheres (B) The final structure of HP35 adsorbed onto HW-Gra surface. Time evaluations of the ratios of (C) the α -helical segment, (D) remaining hydrogen bonds and (E) native protein contacts, Q , of HP35 upon binding to LW-Gra.

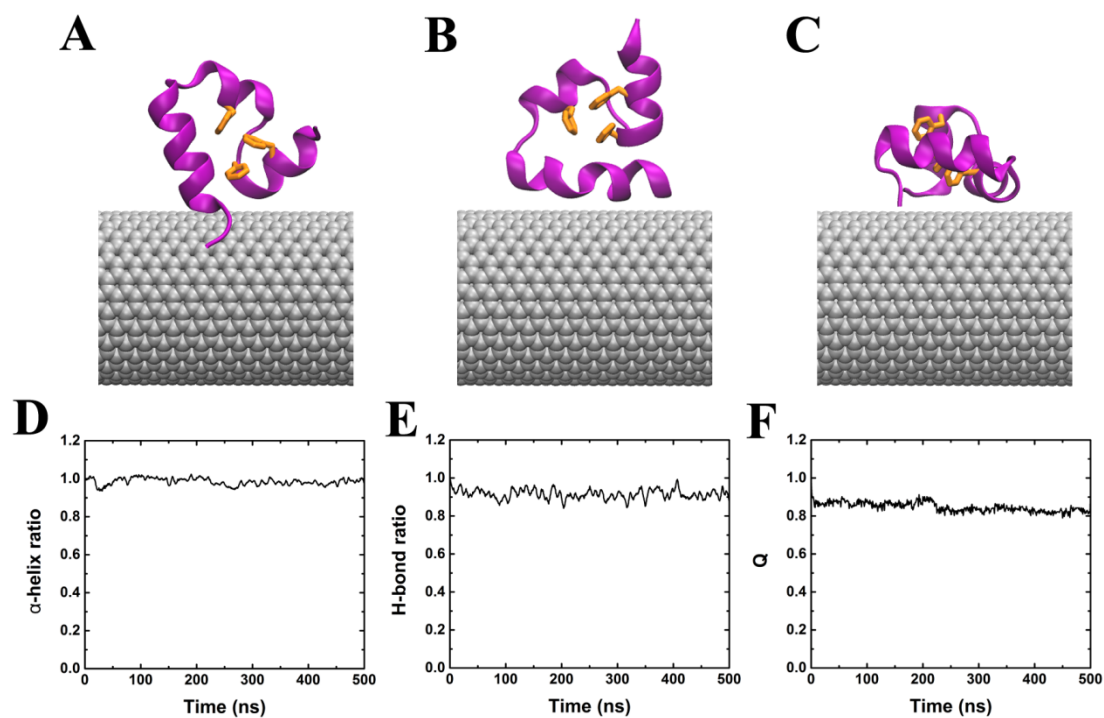


Figure S4. (A-C) Final binding structures of HP35 binding to CNT surface from three 500 ns independent trajectories. Time evaluations of the ratios of (C) the α -helical segment, (D) remaining hydrogen bonds and (E) native protein contacts, Q, of HP35 upon binding to CNT. The data in (D)-(F) are averaged over three independent trajectories.

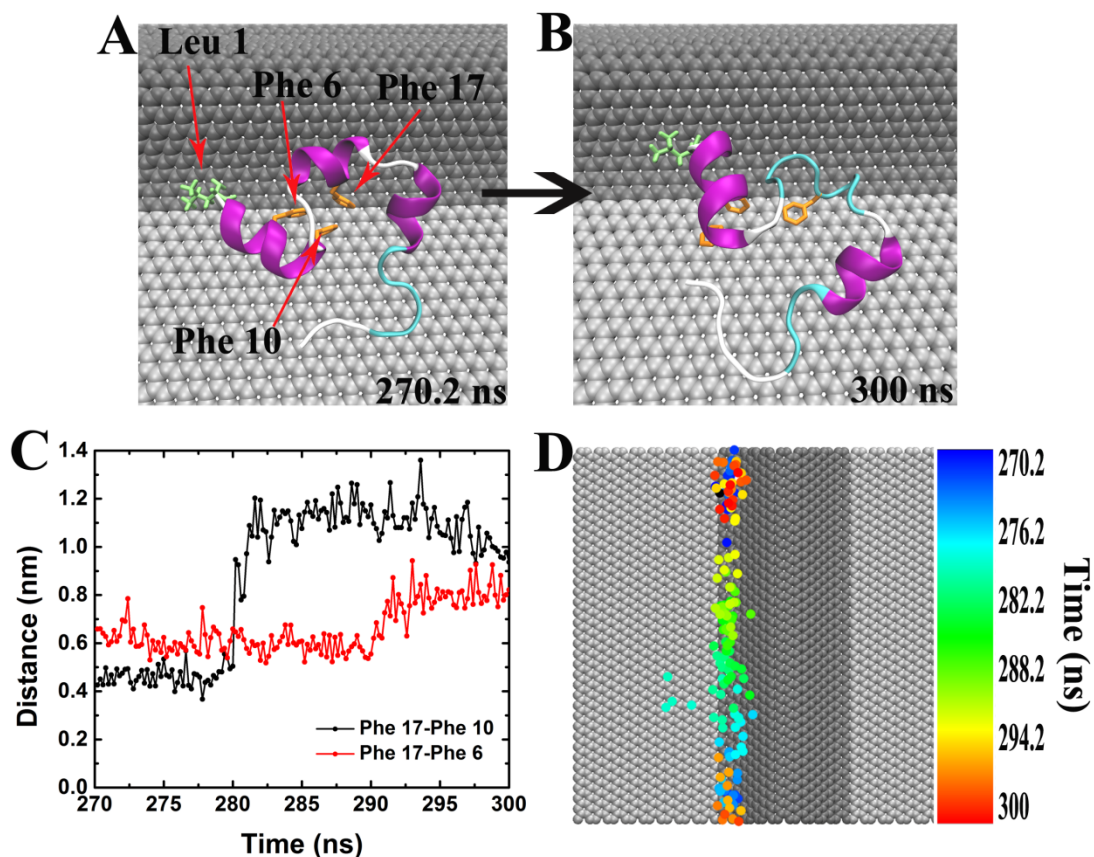


Figure S5. (A-B) Two representative snapshots from traj-2 showing how HP35 unfolds at the winkle corner. (C) Time evaluation of the distance between Phe 17-6 and Phe 17-10. (D) The migration pathway of residue Leu 1 at the corner of winkle from 270.2 to 300 ns.

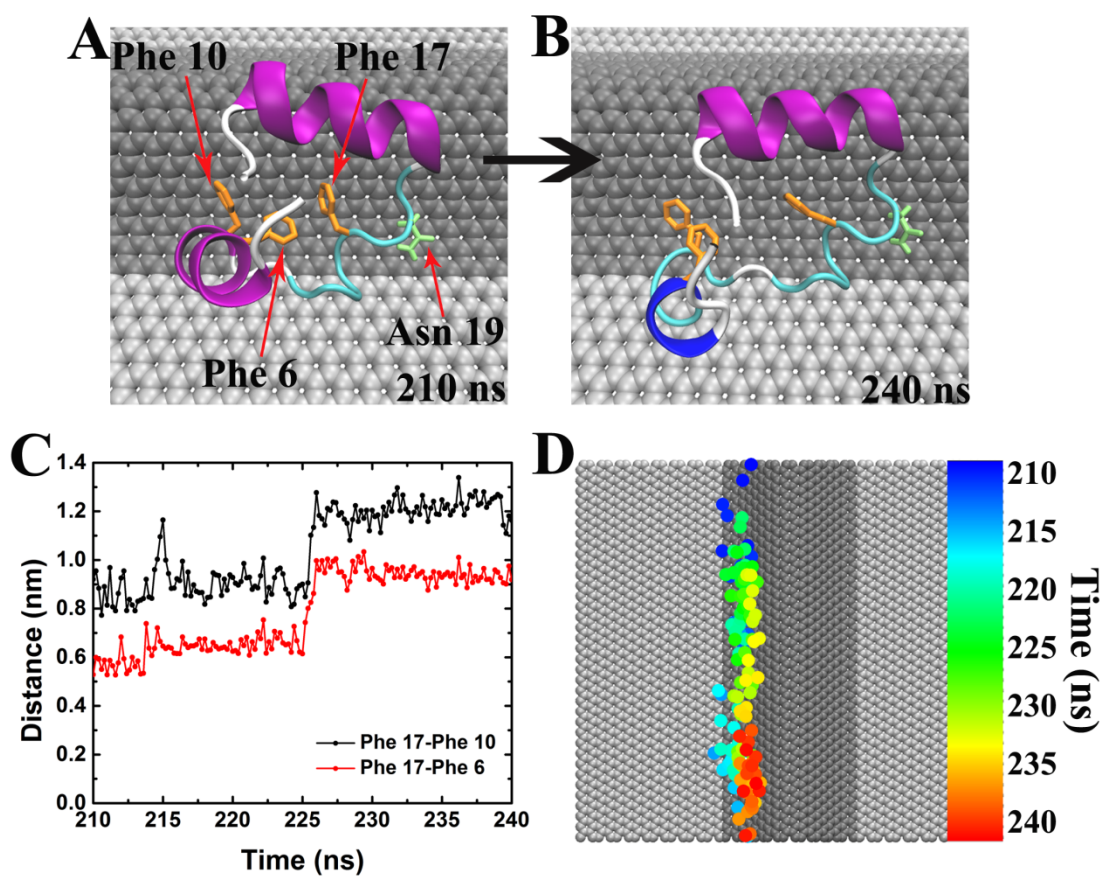


Figure S6. (A-B) Two representative snapshots from traj-3 showing how HP35 unfolds at the winkle corner. (C) Time evaluation of the distance between Phe 17-6 and Phe 17-10. (D) The migration pathway of residue Asn 19 at the corner of winkle from 210 to 240 ns.