Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Structural Influence of Proteins Upon Adsorption to MoS_2 Nanomaterials: Comparison of MoS_2 Force Field Parameters

Zonglin Gu[1], Phil De Luna[2], Zaixing Yang[1], Ruhong Zhou[*1,2,3]

1. School for Radiological and Interdisciplinary Sciences (RAD-X) and Collaborative Innovation Center of Radiation Medicine of Jiangsu Higher Education Institutions, Soochow University, Suzhou, China, 215123

2. Computational Biological Center, IBM Thomas J. Watson Research Center, Yorktown Heights, NY 10598, USA

3. Department of Chemistry, Columbia University, New York, NY 10027, USA

*Corresponding author: ruhongz@us.ibm.com

Table S1. Detailed systems information.

	α-helix/MoS_2				YAP65/MoS_2	HP35/MoS_2
	PA_{10}	PA_{20}	PA_{30}	PA_{40}		
box size	10.39 × 6.74 × 4.00 nm^3				5.00 × 6.00× 8.50 nm^3	6.92 × 6.74 × 5.00 nm^3
material size	10.39 × 6.74 nm^2 (area)				7.90 nm (length)	6.92 × 6.74 nm^2 (area)
water molecule number	7890	7845	7748	7720	7549	6568
counterion number	0	0	0	0	1 chloridion	2 chloridions

Table S2. Systems' information for MoS_2 model in water solvent using two force fields.

	original	**refitted**
box size	3.70 × 3.70 ×3.70 nm^3	3.75 × 3.75 ×3.75 nm^3
water molecule number	1626	1626
counterion number	0	0

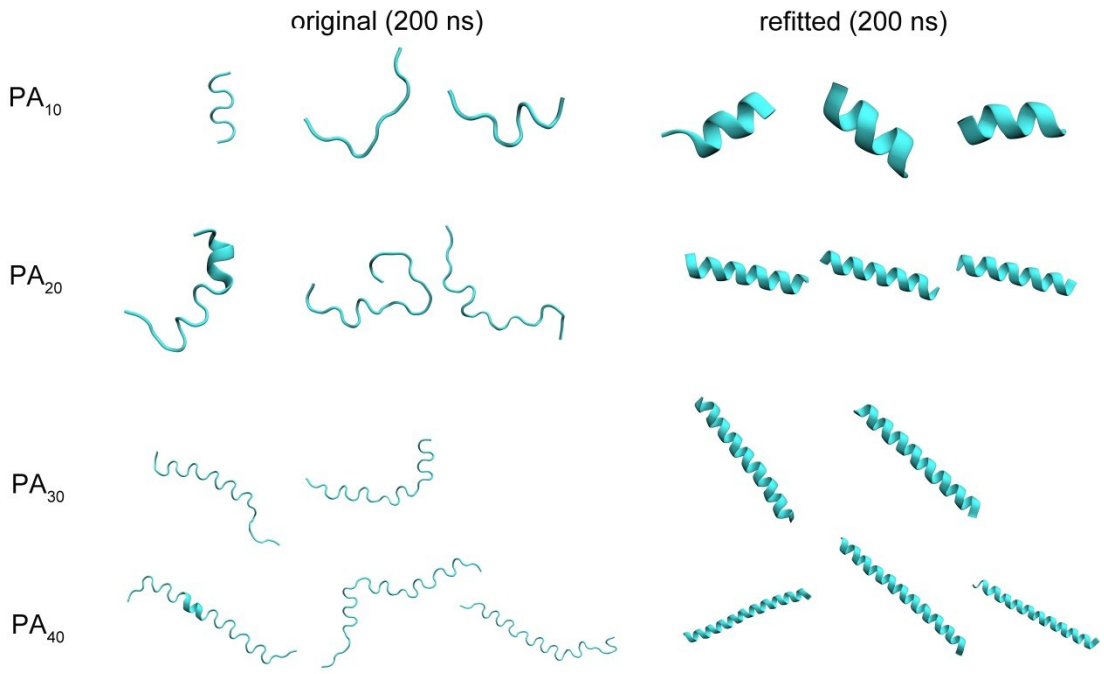

Figure S1. Snapshots of the last frame in three parallel MD trajectories of PA_n binding to MoS_2 using original and refitted MoS_2's force field parameters.

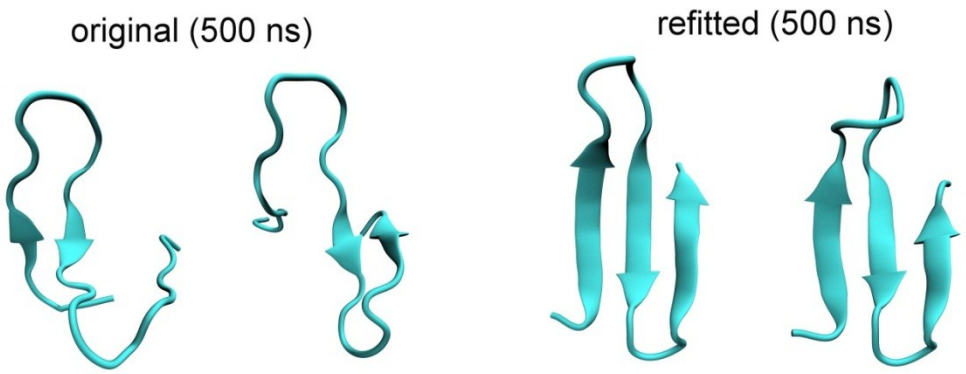

Figure S2. Snapshots of the last frame in two other parallel MD trajectories of YAP65 binding to MoS_2 using original and refitted MoS_2's force field parameters.

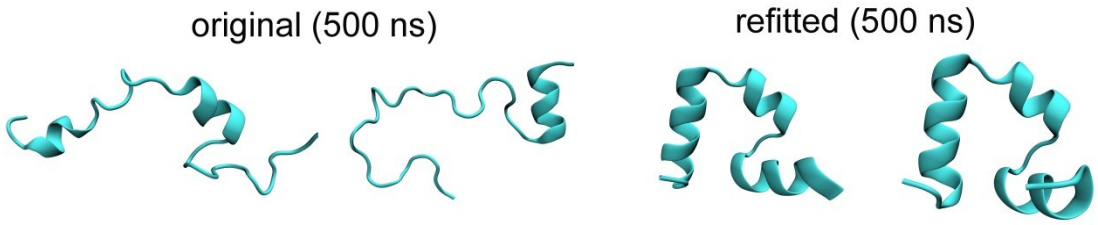

Figure S3. Snapshots of the last frame in two other parallel MD trajectories of HP35 binding to MoS_2 using original and refitted MoS_2's force field parameters.

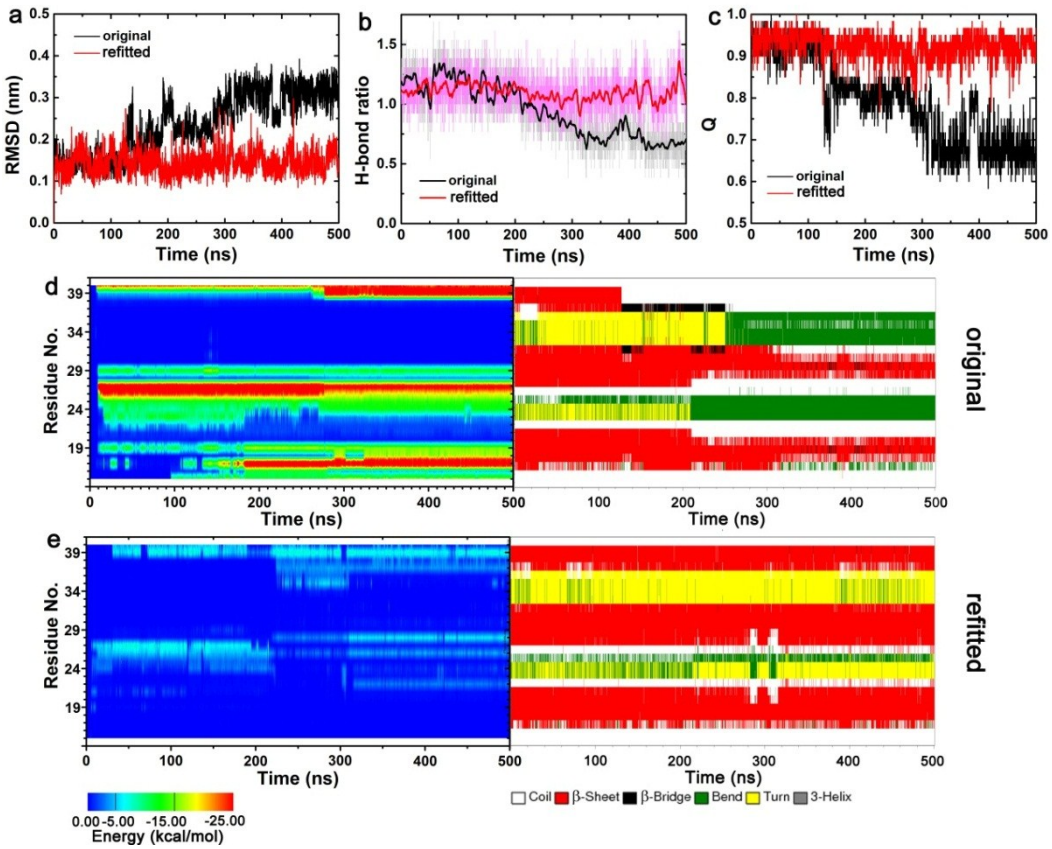

Figure S4. Comparison of YAP65 binding to MoS_2 nanotube using different force field parameters. Root mean square deviation (RMSD, a) of C-α, hydrogen bond (H-bond) ratio (b) and Q value (c) with respect to crystal structure. Time evolution of residue-specific vdW interaction energies (left) of YAP65 on MoS_2 nanotube and secondary structure alteration (right) for original (d) and refitted (e) force fields.

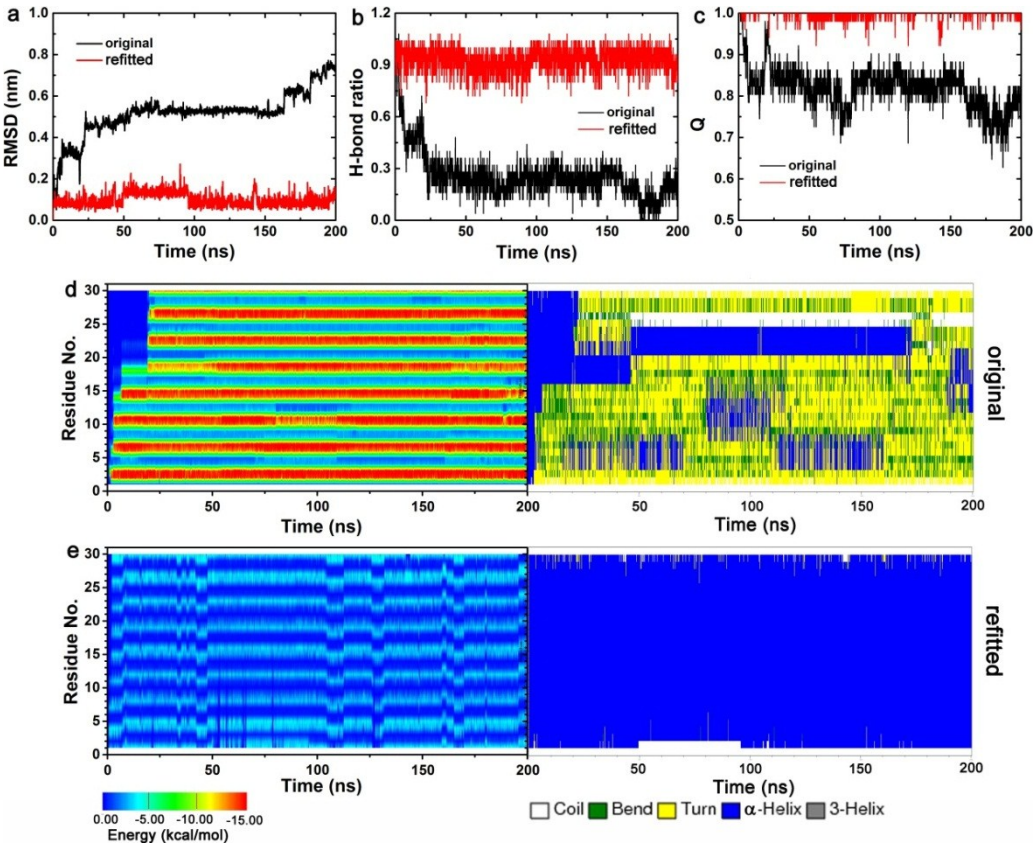

Figure S5. Comparison of PA_{30} binding to MoS_2 nanosheet using different force field parameters. Root mean square deviation (RMSD, a) of C-α, hydrogen bond (H-bond) ratio (b) and Q value (c) with respect to crystal structure. Time evolution of residue-specific vdW interaction energies (left) of PA_{30} on MoS_2 nanosheet and secondary structure alteration (right) for original (d) and refitted (e) force fields.

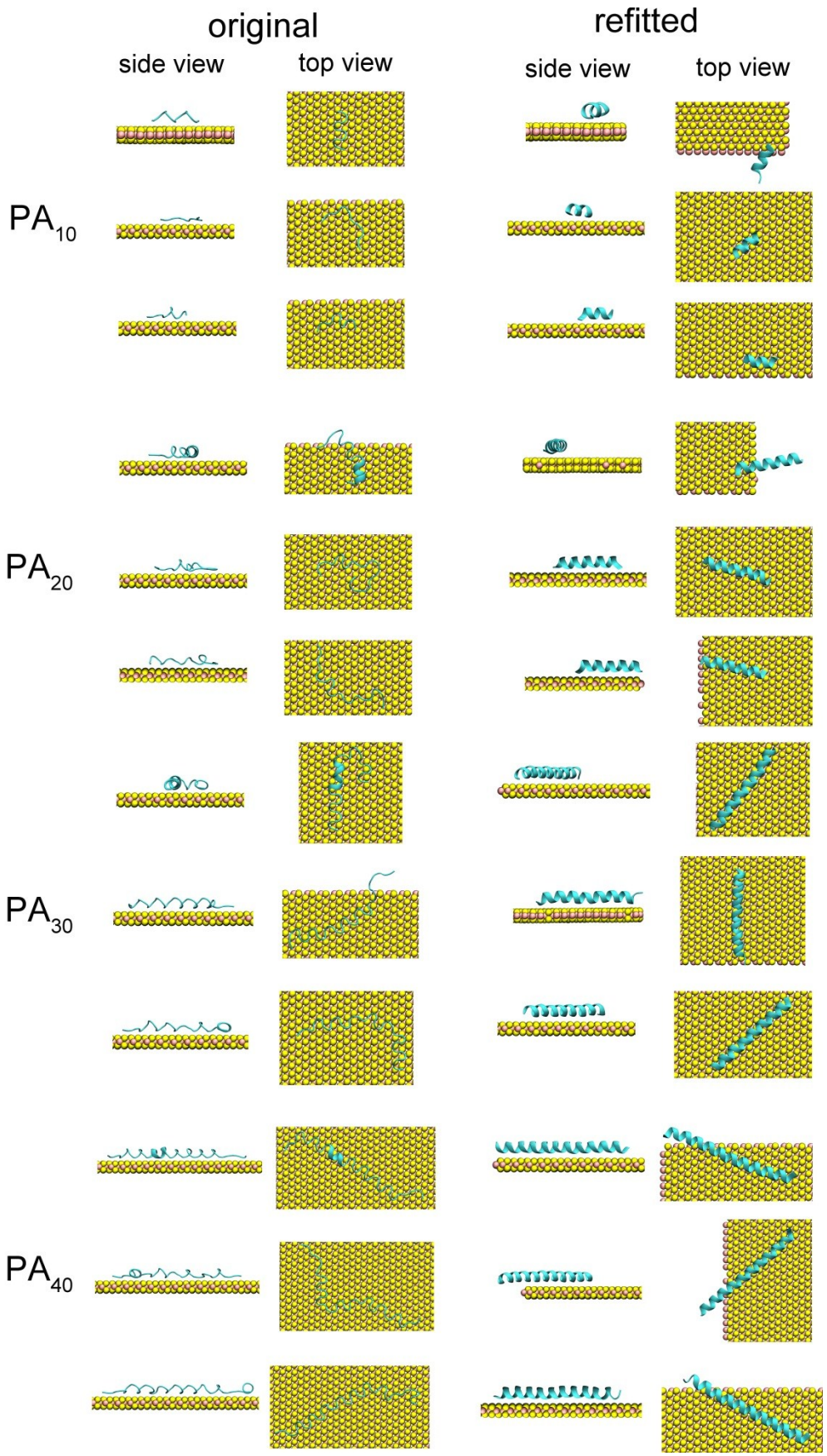

Figure S6. Top and side views of the last snapshots of three parallel PA_n/MoS_2 nanosheet simulations (showing binding events with both protein and nanomaterial) using original and refitted

MoS_2 force field parameters.

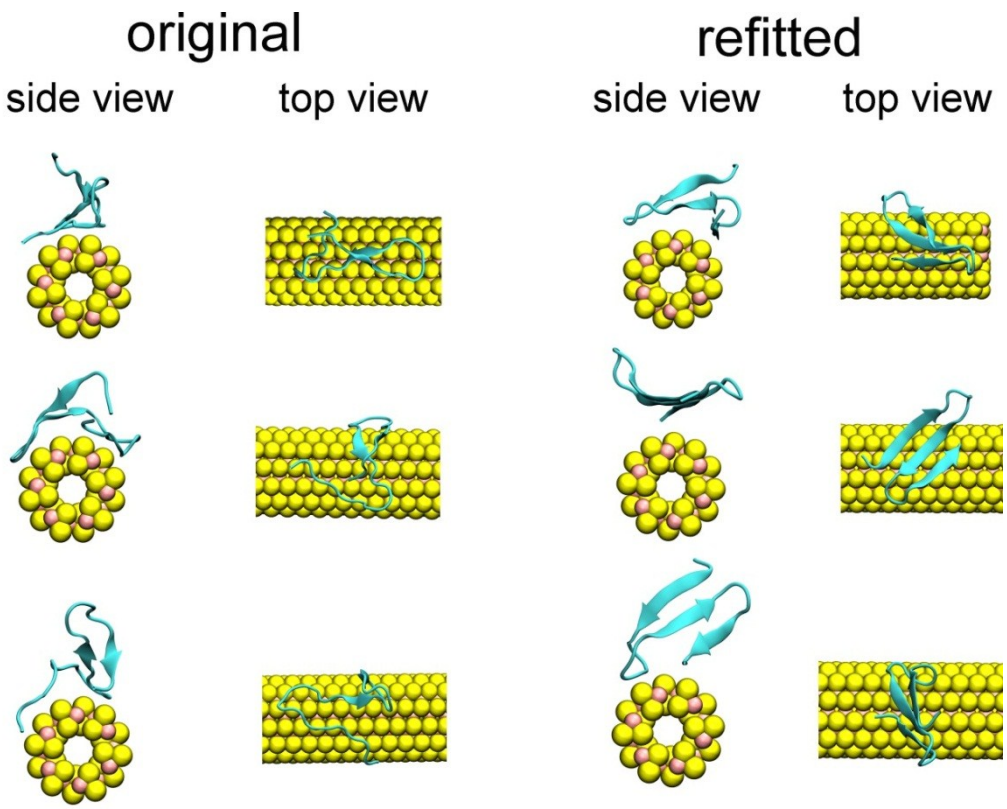

Figure S7. Top and side views of the last snapshots of three parallel YAP65/MoS_2 nanotube simulations (showing binding events with both protein and nanomaterial) using original and refitted MoS_2 force field parameters.

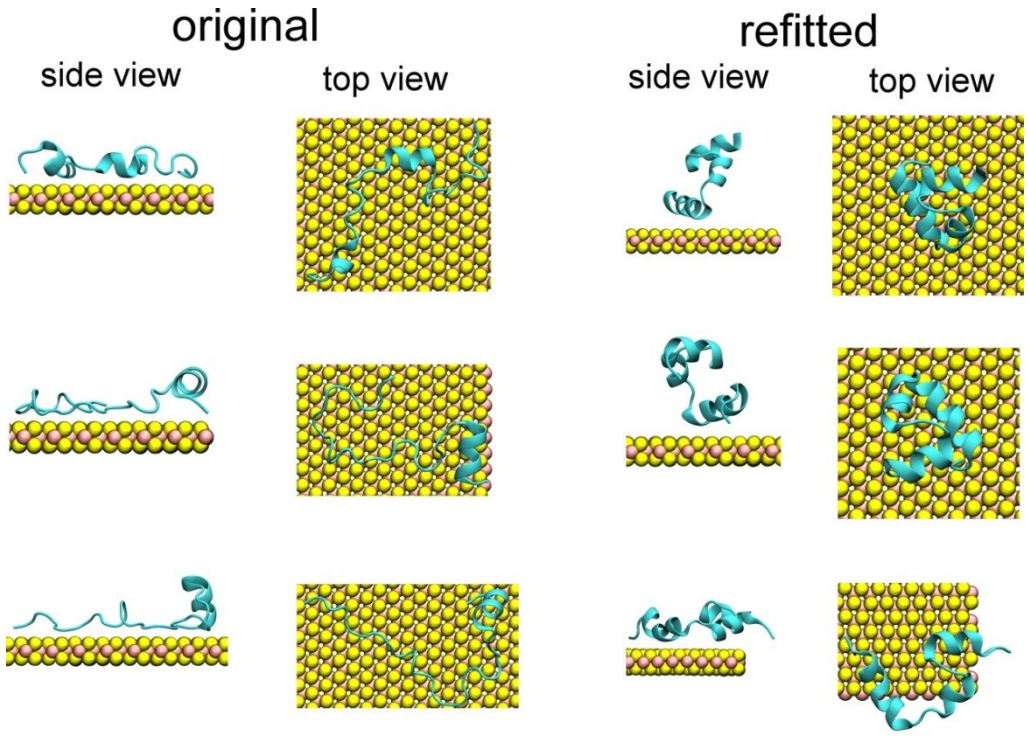

Figure S8. Top and side views of the last snapshots of three parallel HP35/MoS_2 nanosheet simulations (showing binding events with both protein and nanomaterial) using original and refitted MoS_2 force field parameters.

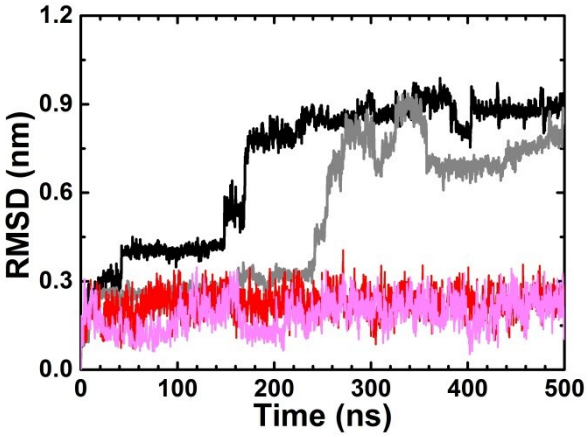

Figure S9. RMSD evolutions of C-α in other four HP35/MoS_2 simulations. Black and gray curves shows the RMSDs using original force field, while the other two represent RMSDs using refitted force field.

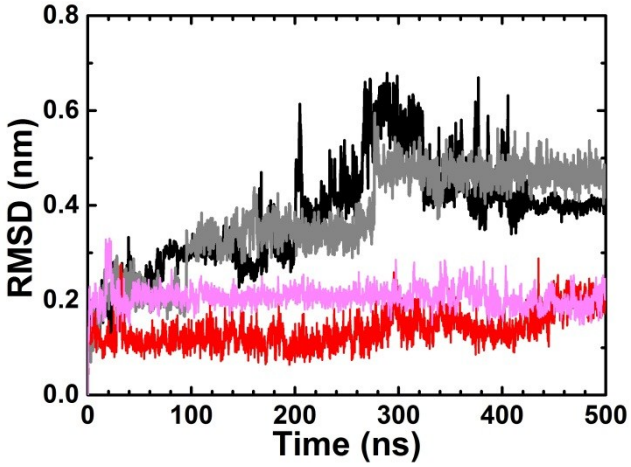

Figure S10. RMSD evolutions of C-α in other four YAP65/MoS_2 simulations. Black and gray curves shows the RMSDs using original force field, while the other two represent RMSDs using refitted force field.

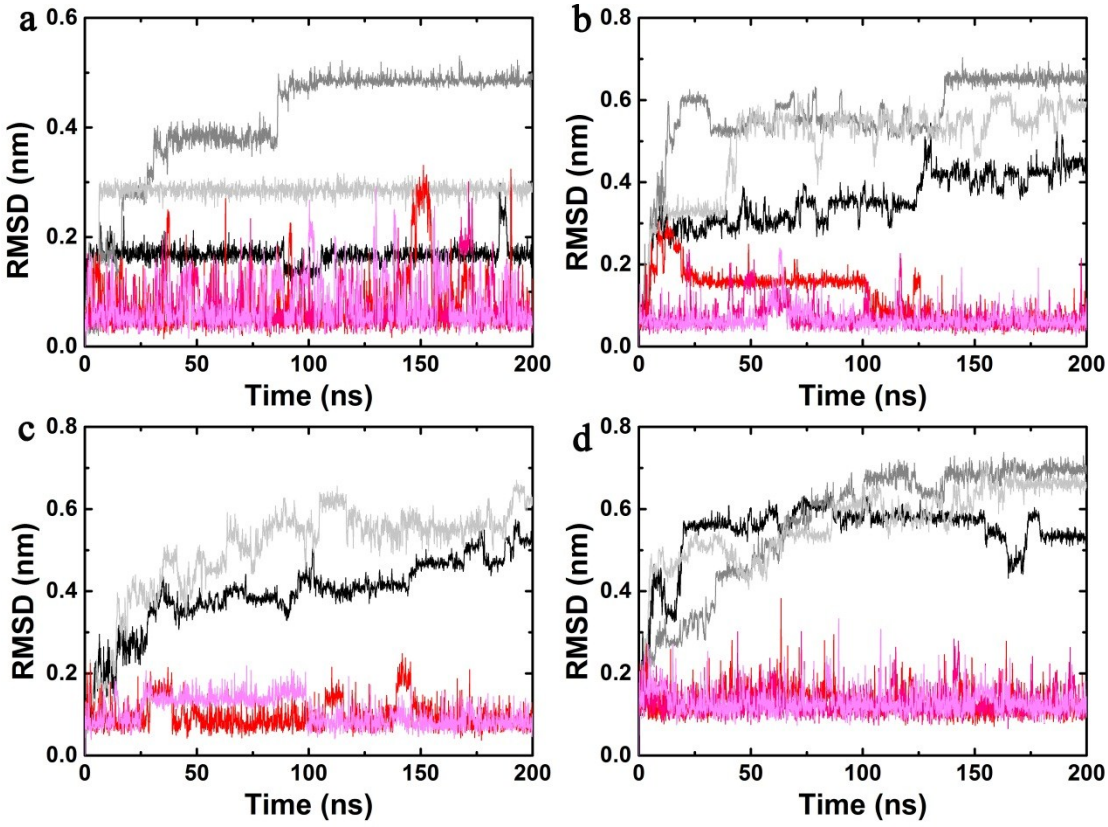

Figure S11. RMSD evolutions of C-α in other polyalanine/MoS_2 simulations. Black, gray and silver curves shows the RMSDs using original force field, while the other ones represent RMSDs using refitted force field.

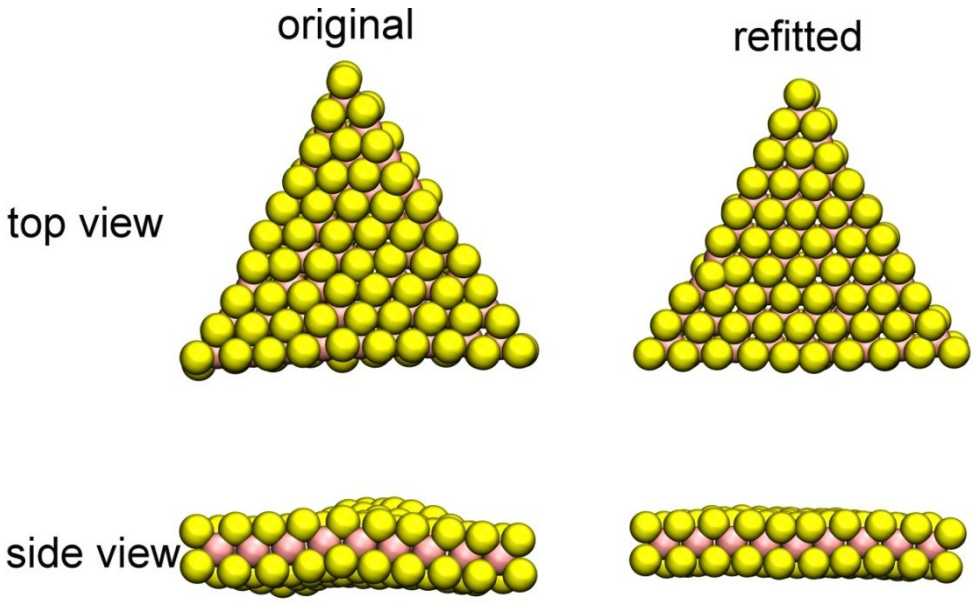

Figure S12. Structures (top and side views) of a representative MoS_2 model performing 10 ns simulations in water solvent using two force fields.