

Supporting Information

Self-Assembly of Diphenylalanine Peptides on Graphene via Detailed Atomistic Simulations

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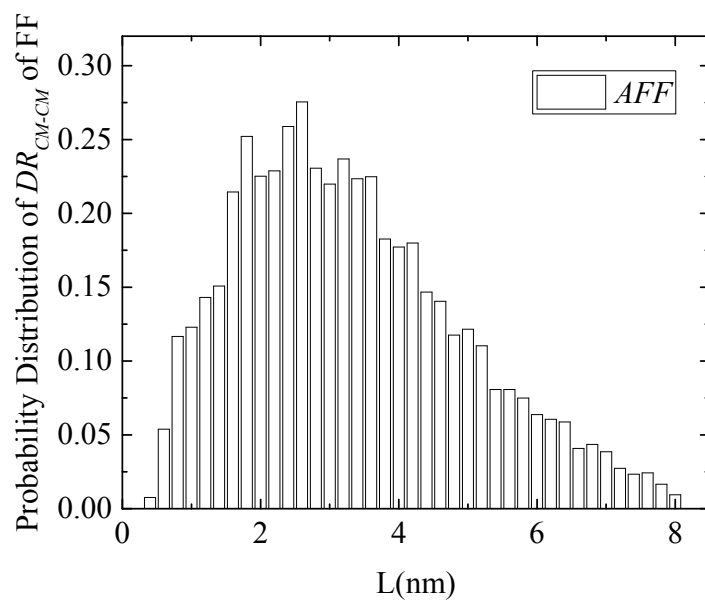


Figure SI-1: Probability distribution of distances among the centers of mass of FF in the initial configuration.

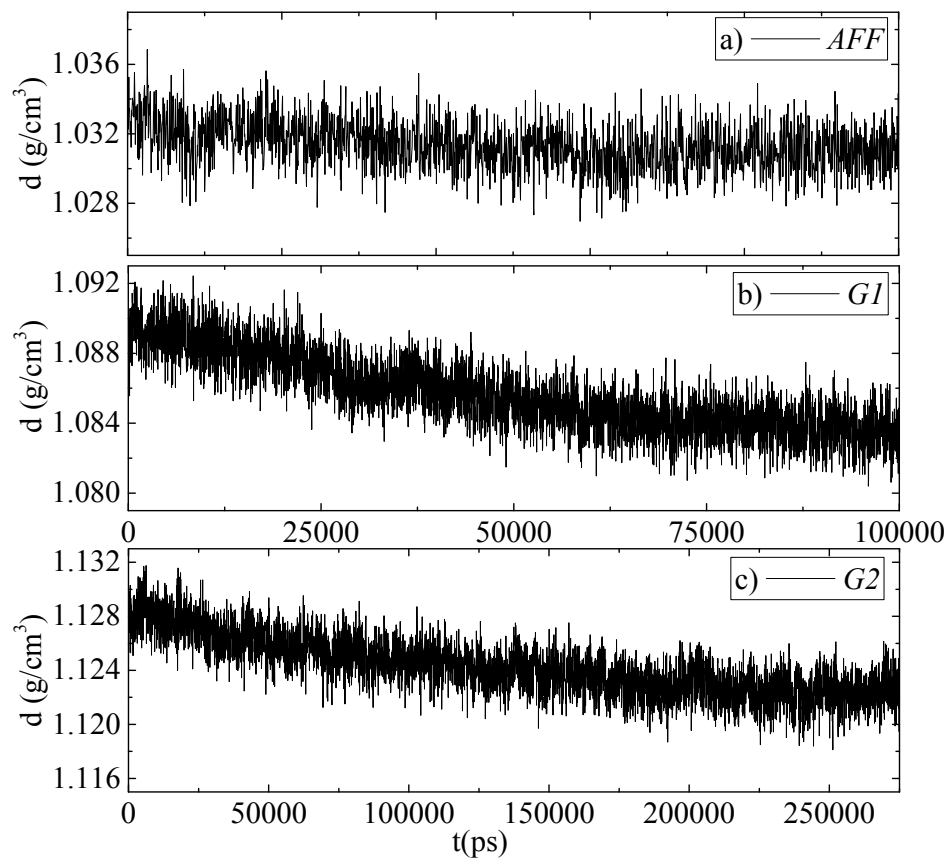


Figure SI-2: System density as a function of time for all three systems.

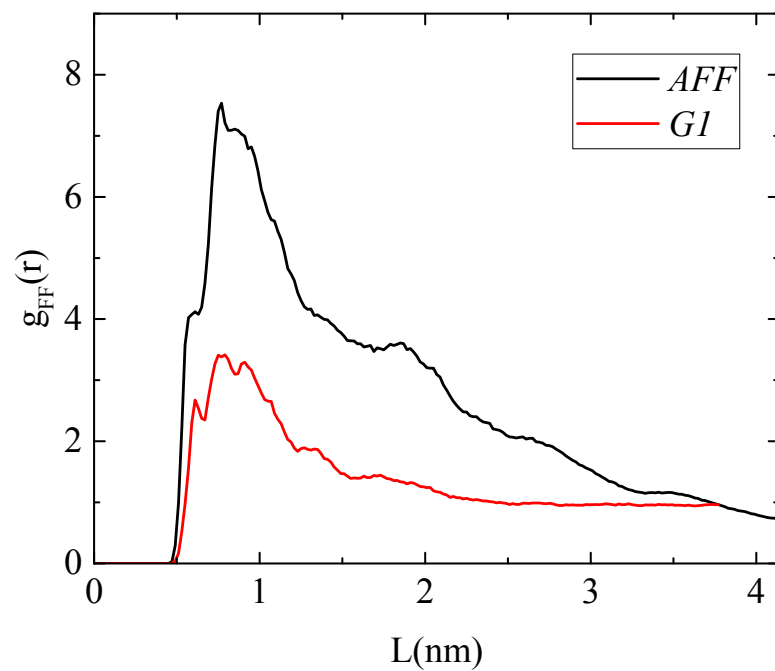


Figure SI-3: Pair radial distribution function between the centers of mass of FF in *AFF* (black curve) and in *GI* coming only from FF molecules whose center of mass is at distance $> 1\text{nm}$ from the graphene surface.