

SUPPLEMENTARY INFORMATION

Polypeptide A9K at Nanoscale Carbon: Simulation Study

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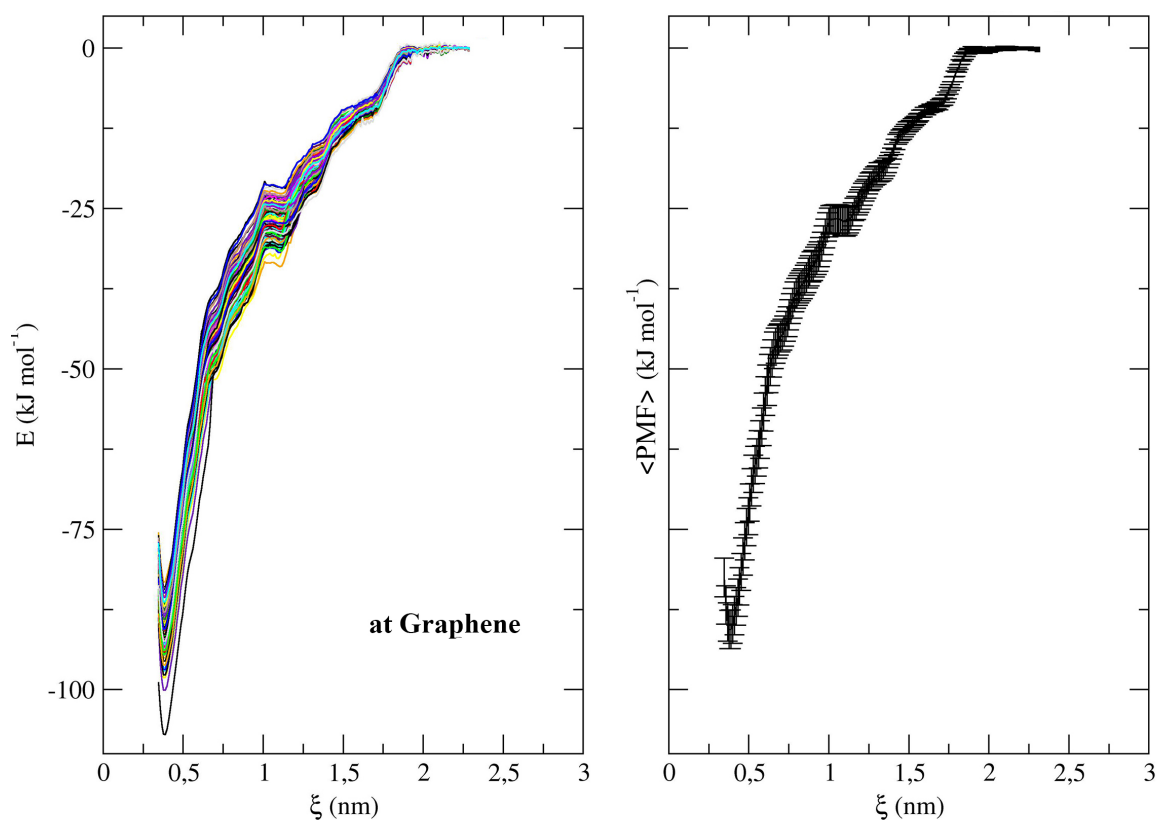


Figure S1. Bootstrap profiles, average values, and standard deviations for the PMF calculation between A9K and graphene. See the manuscript for discussion of the PMF calculation and corresponding methodology in every case.¹

¹ Statistical uncertainty of the PMF is estimated in Gromacs using bootstrap analysis. Bootstrapping is a resampling technique that can be applied to estimate the uncertainty of a quantity, which is computed from a large set of observations. The idea of bootstrapping is to estimate a probability distribution using the n observations (in our case $n=200$) and subsequently generate new random sets of n hypothetical observations, based on the estimated distribution. Each of the set of n hypothetical observations is used to calculate a hypothetical value for PMF (the color curves at left panels). The uncertainty in PMF is then given by the standard deviation of the hypothetical values for PMF (shown at right panels). For a detailed introduction into the bootstrap technique, we refer to the paper 10.1021/ct100494z.

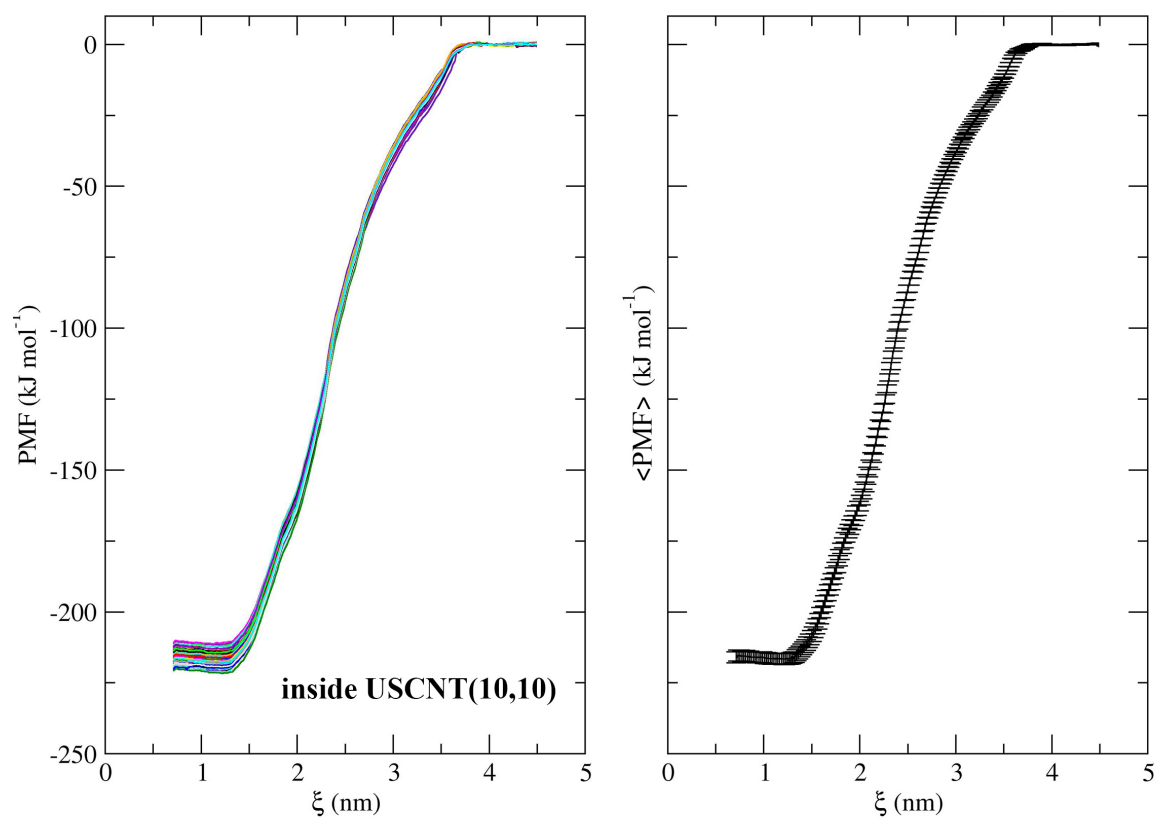


Figure S2. Bootstrap profiles, average values, and standard deviations for the PMF calculation between A9K and the (10,10) USCNT. A9K is inside USCNT. See the manuscript for discussion of the PMF calculation and corresponding methodology in every case.

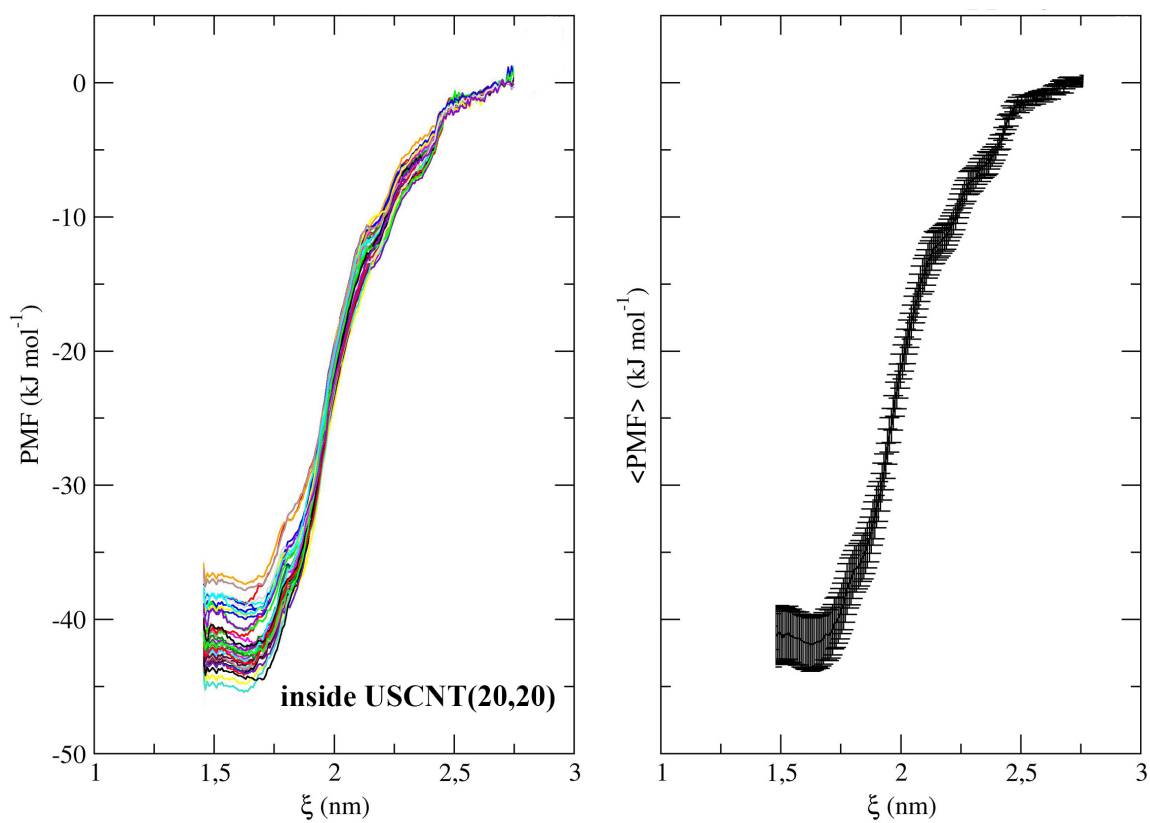


Figure S3. Bootstrap profiles, average values, and standard deviations for the PMF calculation between A9K and the (20,20) USCNT. A9K is inside USCNT. See the manuscript for discussion of the PMF calculation and corresponding methodology in every case.

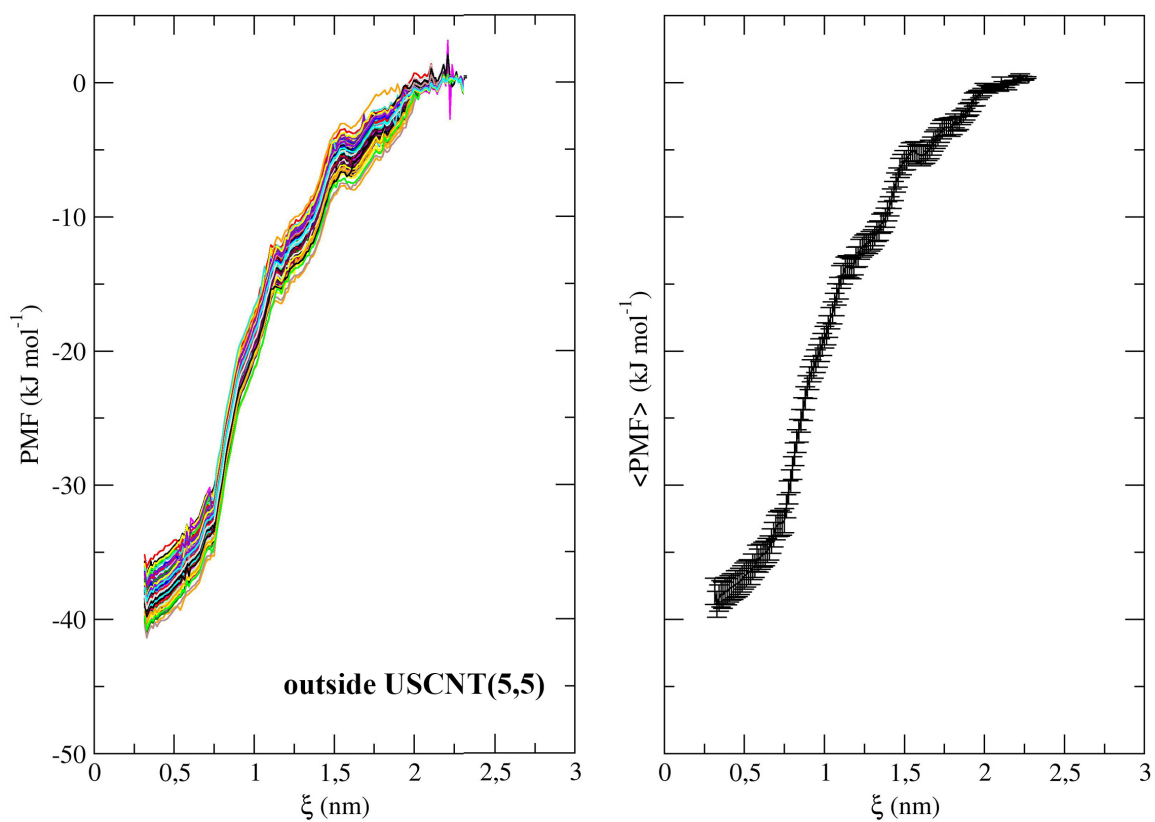


Figure S4. Bootstrap profiles, average values, and standard deviations for the PMF calculation between A9K and the (5,5) USCNT. A9K is outside USCNT. See the manuscript for discussion of the PMF calculation and corresponding methodology in every case.

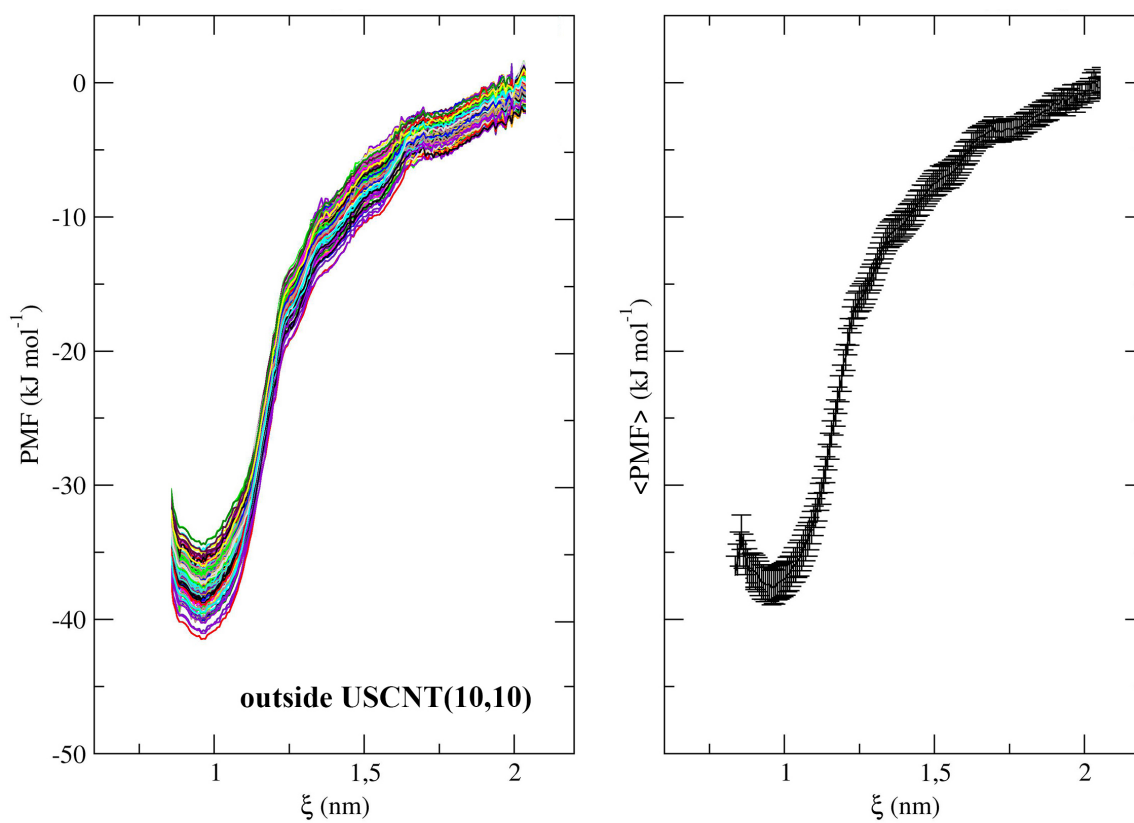


Figure S5. Bootstrap profiles, average values, and standard deviations for the PMF calculation between A9K and the (10,10) USCNT. A9K is outside USCNT. See the manuscript for discussion of the PMF calculation and corresponding methodology in every case.

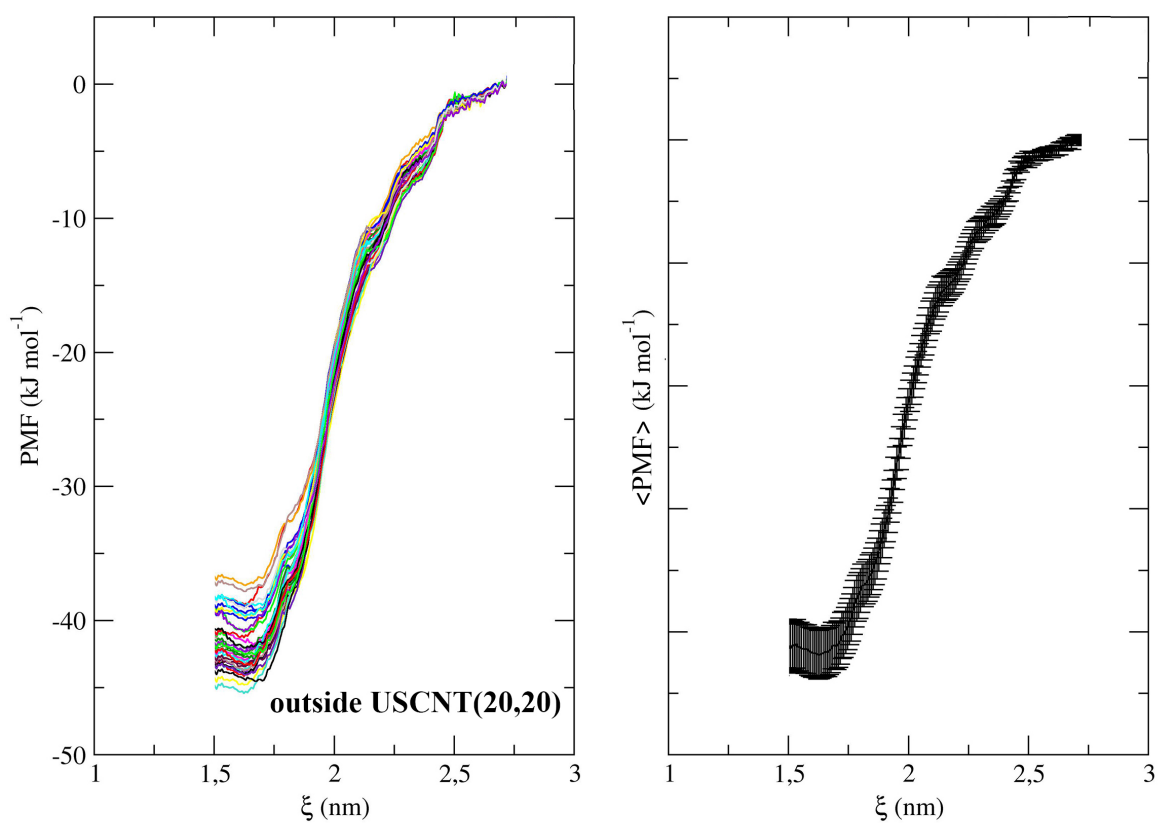


Figure S6. Bootstrap profiles, average values, and standard deviations for the PMF calculation between A9K and the (20,20) USCNT. A9K is outside USCNT. See the manuscript for discussion of the PMF calculation and corresponding methodology in every case.

Systems	ΔG (kJ mol ⁻¹)	k_a
A9K inside CNT(10,10)	-217	3.66×10^{36}
A9K inside CNT (20,20)	-42	1.19×10^7
A9K outside CNT (5,5)	-39	3.73×10^6
A9K outside CNT (10,10)	-38	2.53×10^6
A9K outside CNT (20,20)	-42	1.19×10^7
A9K on graphene	-91	2.15×10^{15}

Table S1: Binding free energy (in kJ mol⁻¹) and the corresponding binding constants for each investigated system.