

# Understanding the Role of Hydrophobic Patches in Protein Disaggregation

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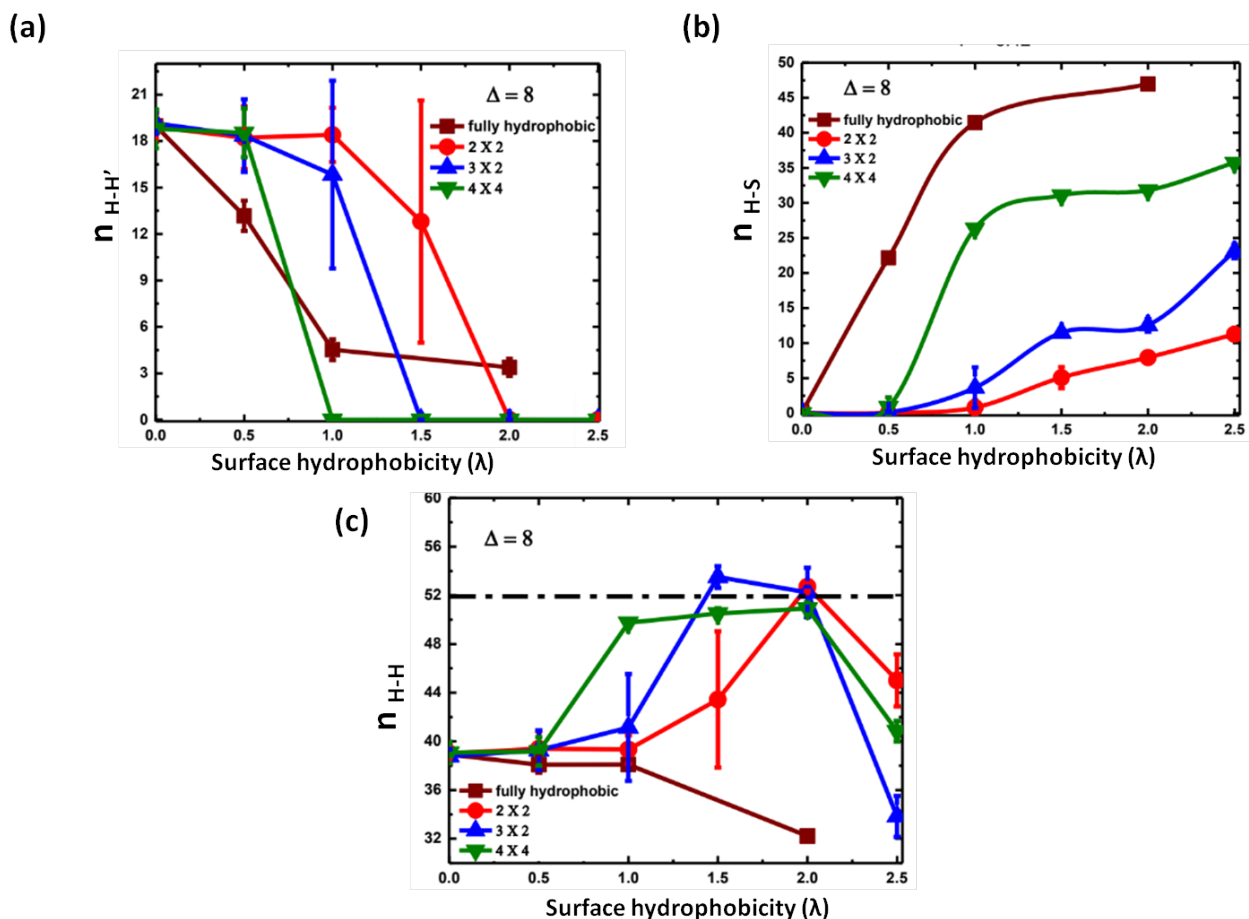


Fig 1: Effect of surface hydrophobicity ( $\lambda$ ) on disaggregation of 42mer HP proteins at  $T^* = 0.42$  on different surface patterns when  $\Delta = 8$  and  $\epsilon_{H-H'} = -1$  (concentrated regime). The behavior on a fully (homogeneous) hydrophobic surface is also graphed for reference a) Average number of inter-protein contacts ( $n_{H-H'}$ ) b) Average number of protein-surface contacts ( $n_{H-S}$ ) c) Average number of intra-protein contacts ( $n_{H-H}$ ) as a function of  $\lambda$ . The dotted line in (c) represents the intraprotein contacts of the protein in dilute regime in bulk.

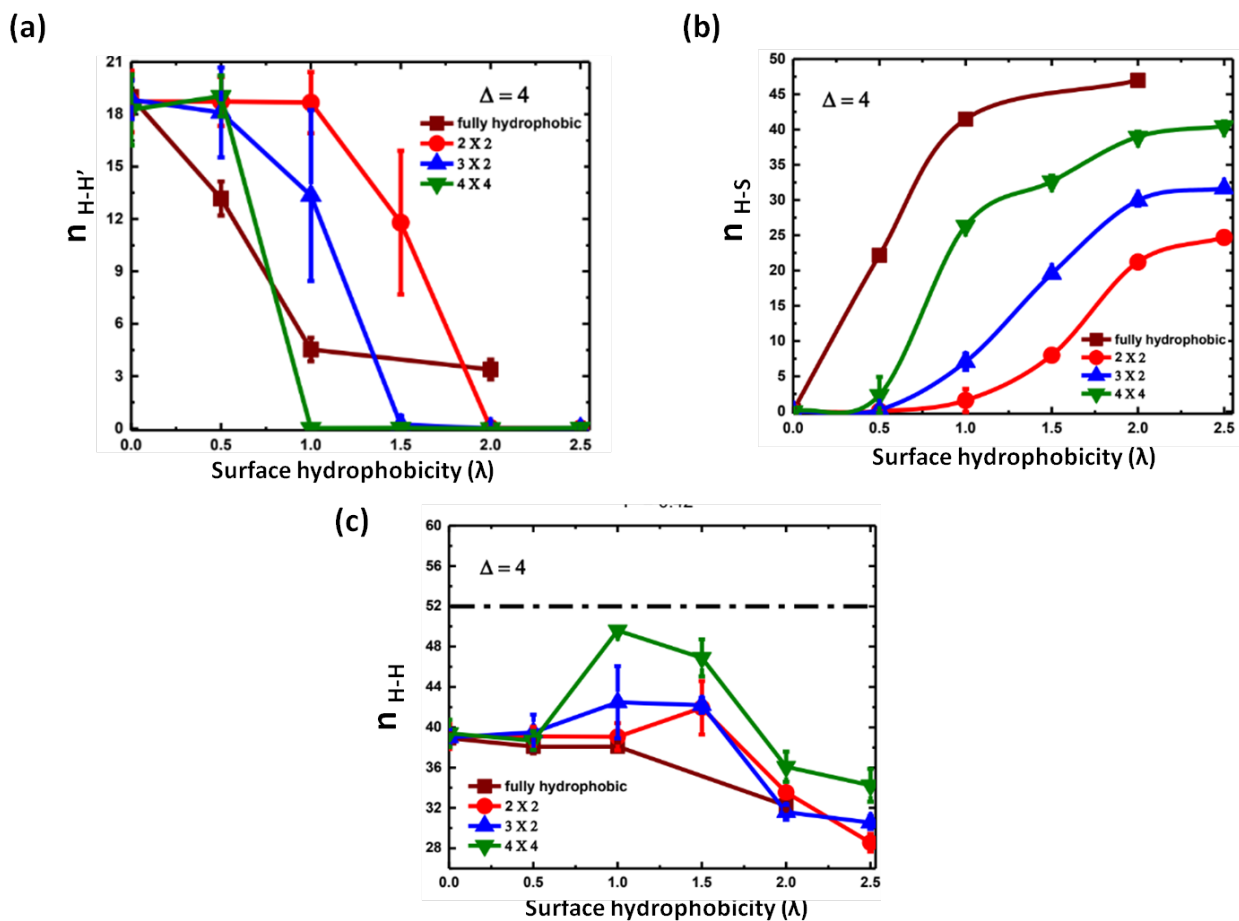


Fig 2: Effect of surface hydrophobicity ( $\lambda$ ) on disaggregation of 42mer HP proteins at  $T^* = 0.42$  on different surface patterns when  $\Delta = 4$  and  $\epsilon_{H-H'} = -1$  (concentrated regime). The behavior on a fully (homogeneous) hydrophobic surface is also graphed for reference  
a) Average number of inter-protein contacts ( $n_{H-H'}$ ) b) Average number of protein-surface contacts ( $n_{H-S}$ ) c) Average number of intra-protein contacts ( $n_{H-H}$ ) as a function of  $\lambda$ . The dotted line in (c) represents the intraprotein contacts of the protein in dilute regime in bulk.

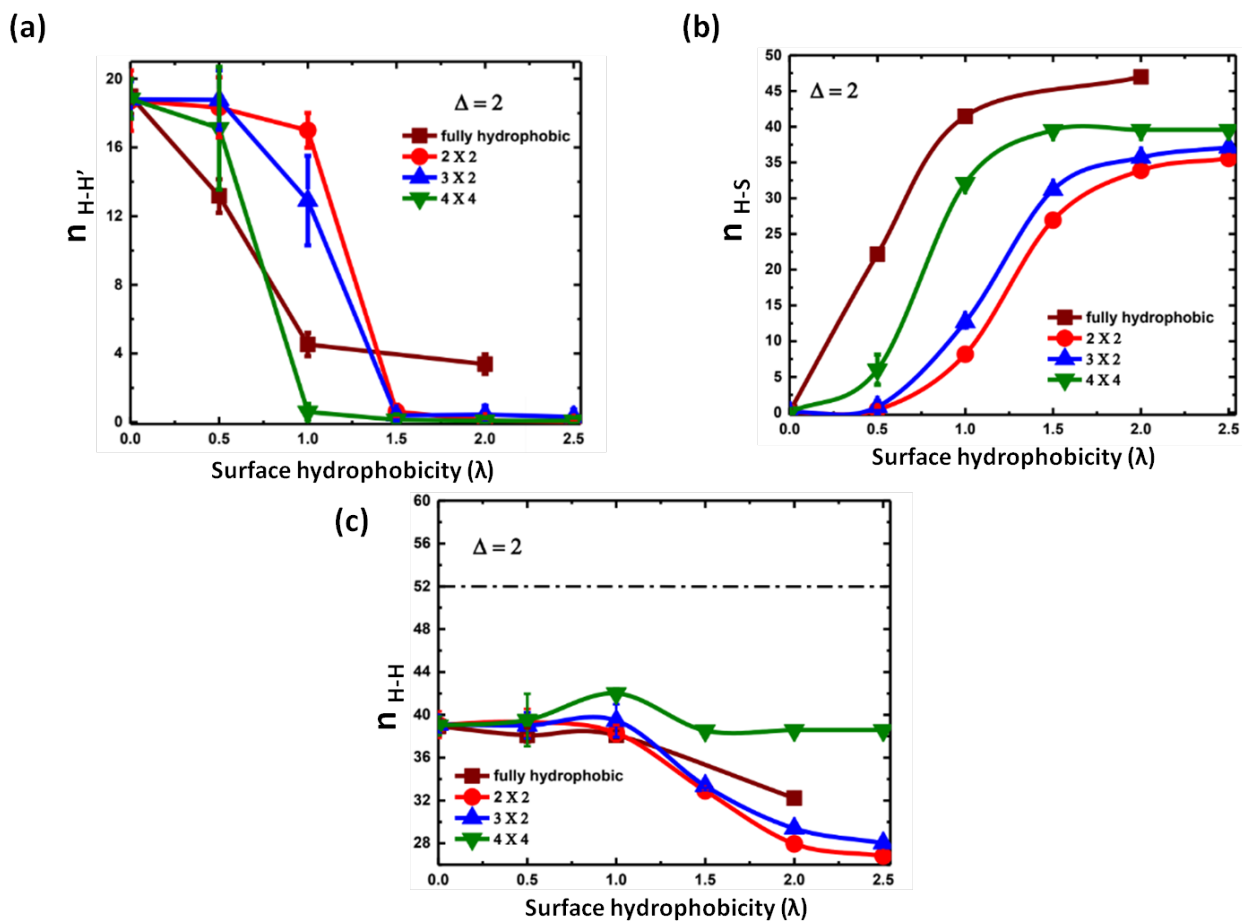


Fig 3: Effect of surface hydrophobicity ( $\lambda$ ) on disaggregation of 42mer HP proteins at  $T^* = 0.42$  on different surface patterns when  $\Delta = 2$  and  $\epsilon_{H-H'} = -1$  (concentrated regime). The behavior on a fully (homogeneous) hydrophobic surface is also graphed for reference a) Average number of inter-protein contacts ( $n_{H-H'}$ ) b) Average number of protein-surface contacts ( $n_{H-S}$ ) c) Average number of intra-protein contacts ( $n_{H-H}$ ) as a function of  $\lambda$ . The dotted line in (c) represents the intraprotein contacts of the protein in dilute regime in bulk.

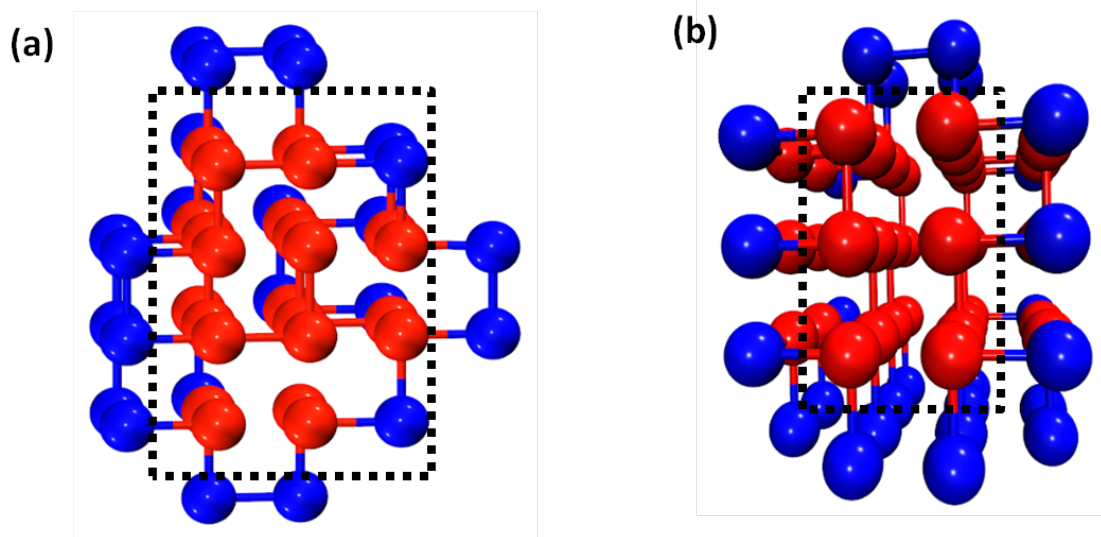


Fig 4: Folded state (native) of the two model HP proteins a) 48 mer HP protein with a native state energy of  $-34\epsilon_{H-H}$  with 10 hydrophobic groups exposed in an asymmetric manner b) 64 mer HP protein with a native state energy of  $-56\epsilon_{H-H}$  with 6 hydrophobic groups exposed in a  $3 \times 2$  manner. Hydrophobic and Polar groups are represented by red and blue beads respectively

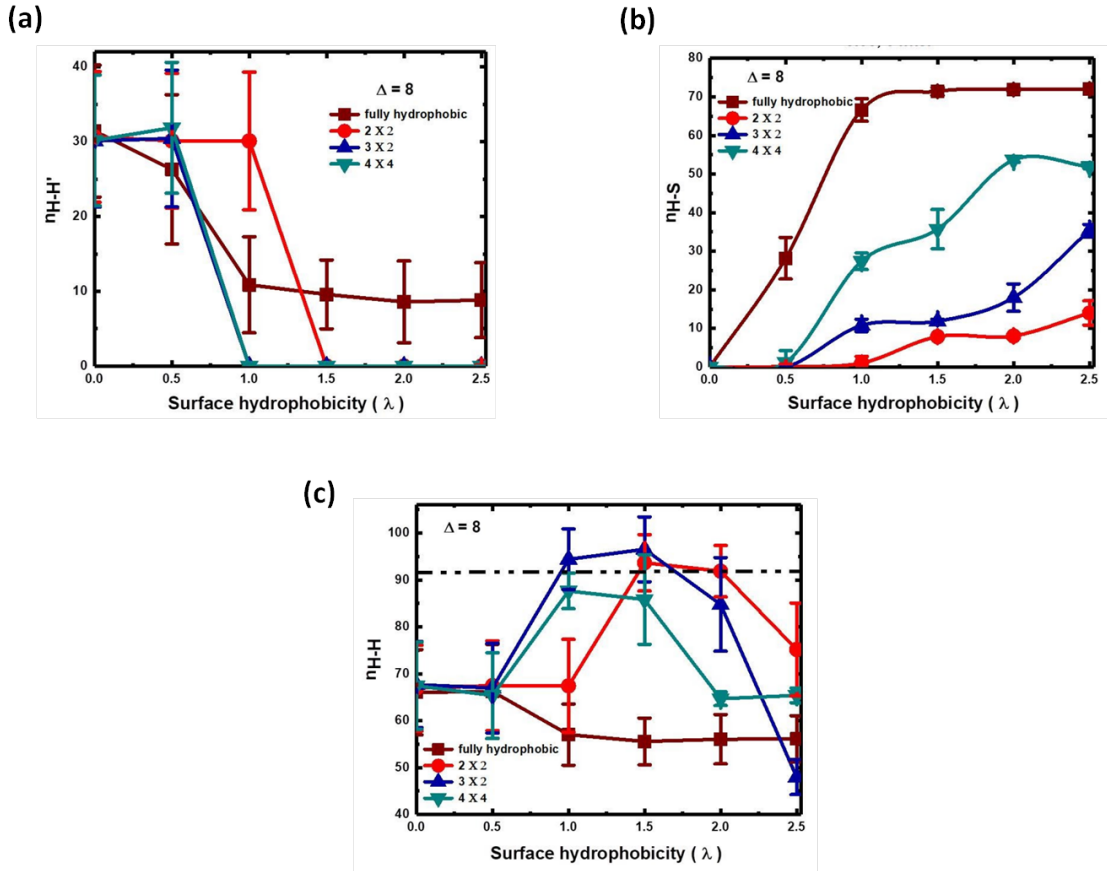


Fig 5: Effect of surface hydrophobicity ( $\lambda$ ) on disaggregation of 64mer HP proteins at  $T^* = 0.38$  on different surface patterns when  $\Delta = 8$  and  $\epsilon_{H-H'} = -1$  (concentrated regime). The behavior on a fully (homogeneous) hydrophobic surface is also graphed for reference  
a) Average number of inter-protein contacts ( $n_{H-H'}$ ) b) Average number of protein-surface contacts ( $n_{H-S}$ ) c) Average number of intra-protein contacts ( $n_{H-H}$ ) as a function of  $\lambda$ .