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Interplay Between Hydrophobic Effect and Dipole Interactions in Peptide Aggregation SAI GANESAN, SILVINA MATYSIAK, Univ of Maryland-College Park — In the past decade, the development of various coarse-grained models for proteins have provided key insights into the driving forces in folding and aggregation.We recently developed a low resolution Water Explicit Polarizable PROtein coarse-grained Model by adding oppositely charged dummy particles inside protein backbone beads.With this model,we were able to achieve significant α/β secondary structure content,without any added bias.We now extend the model to study peptide aggregation at hydrophobic-hydrophilic interface using elastin-like octapeptides (GV)4 as a model system.A condensation-ordering mechanism of aggregation is observed in water.Our results suggest that backbone interpeptide dipolar interactions,not hydrophobicity,plays a more significant role in fibril-like peptide aggregation.We observe a cooperative effect in hydrogen bonding or dipolar interactions, with increase in aggregate size in water and interface.Based on this cooperative effect, we provide a potential explanation for the observed nucleus size in peptide aggregation pathways.Without dipolar particles,peptide aggregation is not observed at the hydrophilic-hydrophobic interface.Thus,the presence of dipoles,not hydrophobicity plays a key role in aggregation observed at hydrophobic interfaces.

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