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Design & Structural Characterization of Amphiphilic 4-Helix Bundle Peptides Vectorially-Oriented at Soft Interfaces. J.K. Blasie, J. Strzalka, S. Ye, T. Xu, E. Nordgren, S. Satija, I. Kuzmenko, T. Gog, Dept. of Chemistry, Univ. of Pennsylvania, Philadelphia, PA 19104, NIST Center for Neutron Research, National Inst. of Standards & Technology, Gaithersburg, MD 20899, Complex Materials Consortium, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439.

Amphiphilic 4-helix bundle peptides have been designed to incorporate both biological and non-biological cofactors. An ensemble of these peptide-cofactor complexes, vectorially oriented at a soft interface between polar and non-polar media, can provide for the translation of their designed molecular function into a macroscopic material property of the interface. Such amphiphilic 4-helix bundle peptides can also serve as model integral membrane proteins for vectorial incorporation into a lipid bilayer providing a molecular laboratory for the detailed study of structure-function correlations. For example, the mechanism by which anesthetic binding to a designed cavity within its hydrophilic domain modulates the ion channel activity of its hydrophobic domain. Detailed structural studies of these amphiphilic peptides within such non-crystalline ensembles can be performed utilizing an essential combination of x-ray scattering, neutron scattering, and molecular dynamics simulation techniques.