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**Examining the air-water interfacial activity of beta-peptides using molecular simulation and experiment.** CLARK A. MILLER, JUAN J. DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison — Amphiphilic beta-peptides (oligomers of beta-amino acids) are predicted to adsorb at the air-water interface using computer simulation and verified using experiments. Molecular dynamics simulations are used to calculate the free energy of adsorption for different degrees of amphiphilicity and different display of hydrophilic groups. Adsorption of selected peptides is examined by measuring the surface tension of a solution of beta-peptides at different concentrations and agreement with simulation results is found. Simulations show that 2/3 hydrophobic residues lead to favorable adsorption at the air-water interface while 1/3 hydrophobic residues is unfavorable. We analyze changes in the conformational properties and angle with the interface to understand the manner of adsorption. We further investigate the behavior of multiple peptides at the interface using computer simulation and determine the surface pressure and peptide-peptide interactions at the interface.

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