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Effective potential for Folding Protein with Both Alpha and Beta Structures NAN-YOW CHEN, CHUNG-YU MOU, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, R.O.C., ZHENG-YAO SU, National Center for High-performance Computing, Hsinchu, Taiwan, R.O.C. — A coarse-grained off-lattice model that can fold proteins with both helix and sheet structures is proposed. To predict the native structure in a reasonable time, the model has included the essential effects of water in an unbiased effective potential. Two new ingredients, the dipole-dipole interaction and the local hydrophobic interaction, are introduced and are shown to be as crucial as the hydrogen bonding. The model allows successful folding of both helix and sheet structures for a number of proteins and may have provided important hints to the study of protein folding.

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