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Effective potentials for Folding Proteins CHUNG-YU MOU, National Tsing Hua University, Taiwan, NAN-YOW CHEN, Academic Sinica, Taiwan, ZHENG-YAO SU, National Center for High-Performance Computing, Taiwan — A coarse-grained off-lattice model that is not biased in any way to the native state is proposed to fold proteins. To predict the native structure in a reasonable time, the model has included the essential effects of water in an 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 the wild-type sequence of protein G and may have provided important hints to the study of protein folding.

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