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Talk Invited Invited Talk

Anharmonicity, mode-coupling and entropy in a uctuating native protein

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We develop a general framework for the analysis of residue uctuations that simultaneously incorporates anharmonicity and mode-coupling in a unied formalism. We show that both deviations from the Gaussian model are important for modeling the multidimensional energy landscape of the protein Crambin (1EJG) in the vicinity of its native state. The eect of anharmonicity and mode-coupling on the uctuational entropy is on the order of a few kcal/mol.

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[1] O.N. Yogurtcu, M. Gur, and B. Erman. Statistical thermodynamics of residue uctuations in native proteins. J. Chem. Phys., 130(9), 2009.

[2] A. Kabakcioglu, D. Yuret, M. Gur, and B. Erman. Submitted for publication.