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Onsets of Anharmonicity in Protein Dynamics ALEXEI SOKOLOV, JOON HO ROH, The University of Akron, JOSEPH CURTIS, NIST — Dynamics of protein lysozyme at various hydration levels is studied using neutron scattering spectroscopy and molecular dynamic simulations. Two onsets of anharmonicity are observed in the temperature variations of the mean-squared displacements of atoms $<x^2>$. One at $T \sim$100K appears in all samples regardless of hydration level. Based on analysis of experimental and simulations data, we ascribe the onset primarily to methyl group rotation. The second, the well-known dynamical transition at $T \sim$200–230K, is only observed at a hydration level h greater than $\sim$0.2 and is ascribed to the activation of an additional relaxation process. We demonstrate that its variation with hydration correlates well with variation of catalytic activity suggesting that the relaxation process is directly related to the activation of modes required for protein function. Microscopic nature of this relaxation process is discussed.

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