Abstract Submitted
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Protein Dynamics Studied via a Disclination Network Based Approach[1] RAHMI OZISIK, OSMAN BURAK OKAN, Rensselaer Polytechnic Institute, KERRI SCHULTZ, Hudson Valley Community College, ARAVIND RAMMOHAN, Corning Research Center — Protein dynamical transition at ca. 200 K is an elusive collective process by which the time-scale distribution of different relaxations is strongly altered (Okan, Atilgan, Atilgan, Biophysical J. 2009, 97, 2080; Atilgan, Aykut, Atilgan, Biophysical J. 2008, 94, 79). It is now confirmed that the backbone topology during this dynamic transition remains intact and there is no structural phase transition during such a dynamic transition. However, the dynamics of backbone torsional jumps shows a freezing behavior below the transition temperature (Atilgan et al., 2008). In the current work, we map the heavy atoms of proteins onto a disclination network and probe temperature dependent dynamics on such a construct. Using a series of 40 ns molecular dynamics cooling simulations spanning the temperature range of 320 K to 160 K with 10 K increments, we track the dynamics of orientational defect networks. The size distribution and defect lifetimes in the disclination network are shown to be central for the dynamical transition in proteins.

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