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Catching the cold: Can computational modeling explain the physical mechanisms behind cold denaturation CRISTIANO DIAS, University of Western Ontario, TAPIO ALA-NISSILA COLLABORATION, MIKKO KARTTUNEN COLLABORATION — Proteins assume a unique three-dimensional structure under physiological conditions. This structure becomes gradually unstable as temperature is raised or lowered. At about 60°C the ordered structure of proteins becomes unstable. This phenomenon is called denaturation and is also observed at low temperatures, around -20°C. While denaturation at high temperature is well understood, the mechanism behind denaturation at low temperature, i.e. cold denaturation, is still controversial. This mechanism depends strongly on the properties of the solvent in which the protein is immersed, i.e. water. In this talk, I will discuss a simplified model for water that we have recently proposed in the literature (to be published) and a microscopic mechanism for cold denaturation (Phys. Rev. Lett. 100, 118101 (2008)).

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