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Frustration in Condensed Matter and Protein Folding Z. LI, S. TANNER, B. CONROY, F. OWENS, M.M. TRAN, C. BOEKEMA, San Jose State University — By means of computer modeling, we are studying frustration in condensed matter and protein folding, including the influence of temperature and Thomson-figure formation. Frustration is due to competing interactions in a disordered state. The key issue is how the particles interact to reach the lowest frustration. The relaxation for frustration is mostly a power function (randomly assigned pattern) or an exponential function (regular patterns like Thomson figures). For the atomic Thomson model, frustration is predicted to decrease with the formation of Thomson figures at zero kelvin. We attempt to apply our frustration modeling to protein folding and dynamics. We investigate the homogeneous protein frustration that would cause the speed of the protein folding to increase. [1] Increase of protein frustration (where frustration and hydrophobicity interplay with protein folding) may lead to a protein mutation. [2] Research is supported by <u>WiSE@SJSU</u> and AFC San Jose.

[1] Contessoto *et al*, Proteins **81** 1727–1737 (2013).

[2] Oliveira, L C et al, Chem Phys **125** 084904-1-7 (2006).

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