Abstract Submitted
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Vibrational Dynamics of Atoms in Proteins[1] DERYA VURAL, HENRY GLYDE, University of Delaware — Biological macromolecules expand with increasing temperature and this dynamic expansion is associated with the onset of function. The expansion is typically caused by thermal vibration and thermal diffusion of atom in the proteins. The expansion is usually characterized by the mean square vibrational displacement (MSD), $\langle u^2 \rangle$, of specific atoms such as hydrogen within the macromolecules. We show that the observed expansion and change in slope of $\langle u^2 \rangle$ with temperature at a dynamical transition temperature, T_D, can be reproduced within a simple model of the dynamics, an atom vibrating in an anharmonic potential, $V(u)$. Only atomic vibration is incorporated, and given $V(u)$, only the temperature is varied in the model. A simple Gaussian potential or a potential containing a hard wall is particularly effective in producing a significant change in the slope of $\langle u^2 \rangle$ with temperature around T_D as is observed.

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