Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

**Structural and functional allostery wiring diagrams in GroEL/GroES**[1] RIINA TEHVER, JIE CHEN, D. THIRUMALAI, University of Maryland — Repeated cycling between distinct allosteric states is required for the functions of numerous biological nanomachines. Determining the specific residues that are responsible for transmitting allosteric signals is needed to understand their operation. Using structural perturbation analysis and evolutionary correlations of mutations of residues, we determine networks of key residues in molecular chaperonin GroEL and its cochaperonin GroES. GroEL is a molecular machine that rescues aggregation-prone misfolded proteins. Its functional cycle consists of a series of large-scale allosteric transitions between the T, R, R' and R" states. The corresponding structural rearrangements facilitate substrate protein capture, refolding, and release. The networks of residues we find provide a microscopic foundation for the cooperativity of the allosteric transitions and a linkage between substrate protein binding and ATPase activity of GroEL.

[1]RT is a National Institute of General Medical Sciences postdoctoral fellow (1F32GM082009). DT is grateful to the NIH (1R01GM067851-01) and the AF Office of Scientific Research (FA9550-07-1-0098).

Riina Tehver
University of Maryland

Date submitted: 19 Nov 2008 Electronic form version 1.4