

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**Ligand Binding Stability and Site Specific Chemical Potentials in the Anisotropic Network Model**<sup>1</sup> RAHMI OZISIK, OSMAN BURAK OKAN, Rensselaer Polytechnic Institute, ARAVIND RAMMOHAN, Corning Research Center — Anisotropic network model (ANM) is a quadratic elastic model based on local force balance around each constituent material point. In ANM the potential energy functional is system specific and is built up from the connectivity and spatial distribution of elastic contacts (Atilgan et al., Biophysical J 2001, 80, 505). Because the potential energy functional is readily available in closed form, it becomes possible to derive exact expressions for energetics of the system. Recently, a simple analytical identity has been derived for free energy change associated with bond addition/removal for the Gaussian Network Model (GNM), which is one dimensional analog of ANM (Hamacher, Phys. Rev. E 2011, 84, 016703). In the current work, we generalize this formulation to ANM, and for an arbitrary potential functional which might have an acting force distribution on its constituents. Our formulation gives a complete characterization of site specific chemical potential under an arbitrary time independent force distribution. We correlate the chemical potentials with bond orientational order parameters evaluated at each site. Our results are validated on all-heavy atom networks for 15 ligand bound/unbound protein pairs, and show the decisive role of coordination geometry around each node. We show that local chemical potential is predominantly governed by changes in the bond orientational order.

Rahmi Ozisik

<sup>1</sup>Partial support was provided by NSF Grant No. 1003574 and RPI Rensselaer Polytechnic Institute

Date submitted: 11 Nov 2011

Electronic form version 1.4