Abstract Submitted
for the TSF16 Meeting of
The American Physical Society

Toward ab initio calculations of polymer structure and properties MARIAN MANCIU, SOROUR HOSSEINI, Physics Department, University of Texas at El Paso — In the absence of special symmetries (such as the translational symmetry of a crystal), ab initio calculations are limited to molecules of small sizes, much smaller than a typical polymer. We showed that the energetic and entropic contributions to the partition function of a long polymer can be separated via a variational procedure. This procedure allows the partition function of the polymer to be written as a sum over simpler (and shorter) configurations, such as trains, loops, tails and bridges, occurring with known probabilities, which depend on both their entropy and configuration energy (the later one taking into account the interactions with the rest of the system via a mean field Flory-Huggins approach). Because these configurations are much smaller than the original polymer, the procedure reduces drastically the number of molecules for which the *ab initio* calculations have to be performed.

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Date submitted: 22 Sep 2016 Electronic form version 1.4