Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Depletion induced coil-globule transition of a generic macromolecule: simulations and theory MARTIN BERTRAND, TYLER N. SHENDRUK, University of Ottawa, HENDRICK DE HAAN, University of Ontario Institute of Technology, JAMES L. HARDEN, GARY W. SLATER, University of Ottawa — Entropic depletion forces play a role in the compaction of chromosomal material in simple cells such as bacteria but it remains debatable whether they are sufficient to account for complete chromosome collapse. Using Coarse-Grained Molecular Dynamics simulations we show that depletion induced attractive interactions are sufficient to cause the coil-globule transition of a model chain of supercoiled DNA structural monomers suspended in a bath of smaller generic crowding agents such as proteins. We present a simple theoretical model and quantitatively cast the action of depletants on a generic macromolecular chain as an effective solvent quality: as molecular crowding increases, the radius of gyration goes from its good solvent to globular value via a theta-point and a poor solvent regime. The abrupt collapse of the chain at the predicted volume fraction of depletants is a second-order phase transition. Such coarse-grained simulations may be useful for modelling the effects of molecular crowding on chromosomal DNA in more complex geometries.

Martin Bertrand
University of Ottawa

Date submitted: 15 Nov 2013 Electronic form version 1.4