Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Shape transition in channel- and cavity-confined semiflexible bio-macromolecules[1] PETER CIFRA, TOMAS BLEHA, Polymer Institute, Slovak Academy of Sciences — Stiff macromolecules entrapped in channels or spherical cavities undergo a shape transition on increasing confinement as shown by our investigation using molecular simulations. In channels this weak-to-strong confinement transition leads to extended conformations without the hairpin-like back-folding. In cavities, on decrease of cavity radius, the semiflexible chain in a disordered state starts to organize into the torus. This happens when the extent of confinement reaches the lower bound of macromolecular flexibility given by the minimal radius of chain curvature or the persistence length. As a common rule for both types of confinement the transition to the ordered structures is observed when the radius of cavity or cylindrical channel comes down to the persistence length of macromolecular chain. This simple geometric rule finds its application in various confinement situations of stiff bio-macromolecules either in micro channel experiments or real biophysical situation such as DNA in viral capsids.

[1]Support from APVV-0079-07 is acknowledged.

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Date submitted: 02 Nov 2009 Electronic form version 1.4