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Polymers in Crowded Environment: Globule-coil Transitions and Shape Anisotropy

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We study the flexible polymer macromolecules in a disordered environment with structural obstacles, modeling the protein folding in crowded environment of biological cells. We exploit the model of self-attracting self-avoiding walks on site-diluted percolative lattices in space dimensions d=2, 3. Applying the pruned-enriched Rosenbluth chain-growth method (PERM), we estimate the Θ-transition temperature of globule-coil transition and analyze the influence of stretching force on the polymer folding. We construct the phase diagrams of collapsed and extended states coexistence when varying both the temperature and external stretching force [1]. The influence of structural defects in a disordered environment on the size and shape characteristics of flexible polymers is studied. We numerically estimate rotationally invariant universal quantities such as the averaged asphericity and prolateness of polymer chain configurations. Our results quantitatively reveal the extent of anisotropy of macromolecules due to the presence of structural obstacles.

[1] Blavatska V., Janke W., *Phys. Rev. E* **80**, (2009), p. 051805.