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Free energy cost of localizing a single monomer of a confined polymer

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We describe a simple Monte Carlo simulation method to calculate the free energy cost of localizing a single monomer of a polymer confined to a cavity for a localization site on the inside surface of the confining cavity. The method is applied to a freely-jointed hard-sphere polymer chain confined to cavities of spherical and cubic geometries. In the latter case we consider localization at both the corners and the centers of the faces of the confining cube. We consider cases of end-monomer localization both with and without tethering of the other end-monomer to a point on the surface. We also examine localization of monomers at arbitrary position along the contour of the polymer. We characterize the dependence of the free energy on the cavity size and shape, the localization
position, and the polymer length. The quantitative trends can be understood using standard scaling arguments and use of a simple theoretical model. The relevance of these results to the initial stages of polymer translocation through nanopores and polymer dynamics in porous environments is discussed.

Authors: POLSON, James (University of Prince Edward Island); Mr MCLURE, Zakary (University of Prince Edward Island)

Presenter: POLSON, James (University of Prince Edward Island)

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