

Abstract Submitted  
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**Equilibrium Partitioning of Polymers between Bulk Dilute Solution and Confining Pores**<sup>1</sup> YANWEI WANG, FLEMMING Y. HANSEN, GUENTHER H. PETERS, OLE HASSAGER, Technical University of Denmark — We have developed a novel framework [1] for the description of the steric hindrance effect on polymers that are subject to confining geometries. The two main ingredients are (i) a new computational method, the Confinement Analysis from Bulk Structures (CABS) approach, which enables calculation of the equilibrium partition coefficient (pore-to-bulk concentration ratio) as a function of the confinement size solely based on snapshots of polymer configurations in bulk, and (ii) the definition of a new molecular size parameter, the steric exclusion radius, which permits collapsing all partition coefficient data for different polymers in the weak confinement regime onto a universal curve. Our latest development in extending the CABS method to cylindrical and spherical pores will be presented.

[1] Wang et al. J. Chem. Phys. 128, 124904 (2008); 129, 074904 (2008).

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Yanwei Wang  
Technical University of Denmark

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