

Supporting information for "Excess entropy scaling for the segmental and global dynamics of  
polyethylene melts"

Evangelos Voyiatzis, Florian Müller-Plathe and Michael C. Böhm

Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Center of Smart Interfaces,

Technische Universität Darmstadt, Alarich-Weiss-Strasse 4, D-64287Darmstadt, Germany

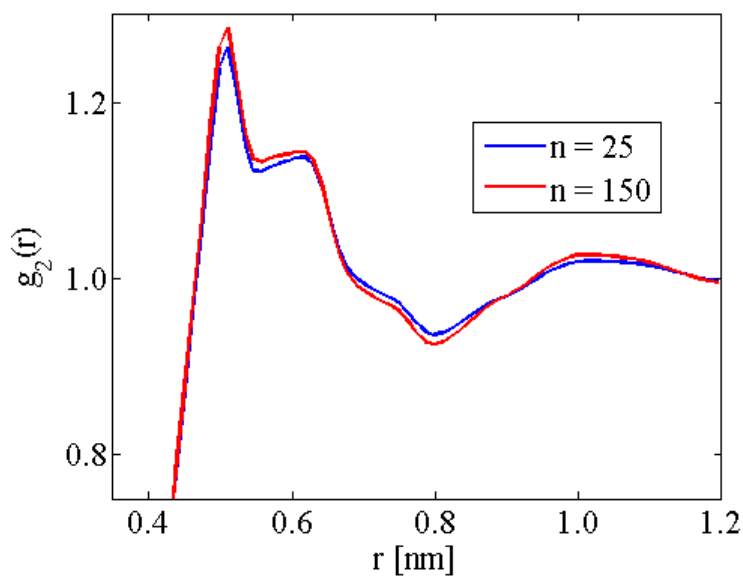


Figure S1. Structure of the pair correlation function  $g_2(r)$  of polyethylene chains at 500 K as a function of the distance  $r$  measured relative to a chosen reference carbon atom. First neighbors on the same chain are excluded.  $g_2(r)$  is presented for two different chain lengths at a pressure of 101.325 kPa.

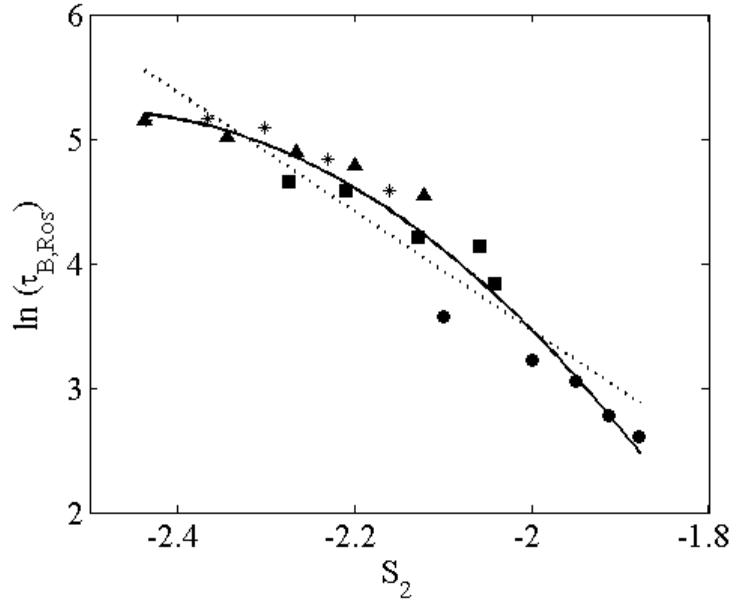


Figure S2. Correlation between the natural logarithm of the bond relaxation time, scaled by the Rosenfeld scheme,  $\tau_{B,Ros}$ , and the pair entropy,  $S_2$ . The dotted line corresponds to the best linear fit  $\ln(\tau_{B,Ros}) = -6.088 - 4.773S_2$  while the solid line to the best fit using the expression  $\ln(\tau_{B,Ros}) = -40.10 - 36.39S_2 - 7.305S_2^2$ . The temperatures and the chain lengths correspond to the same setup as employed in the other correlation schemes.

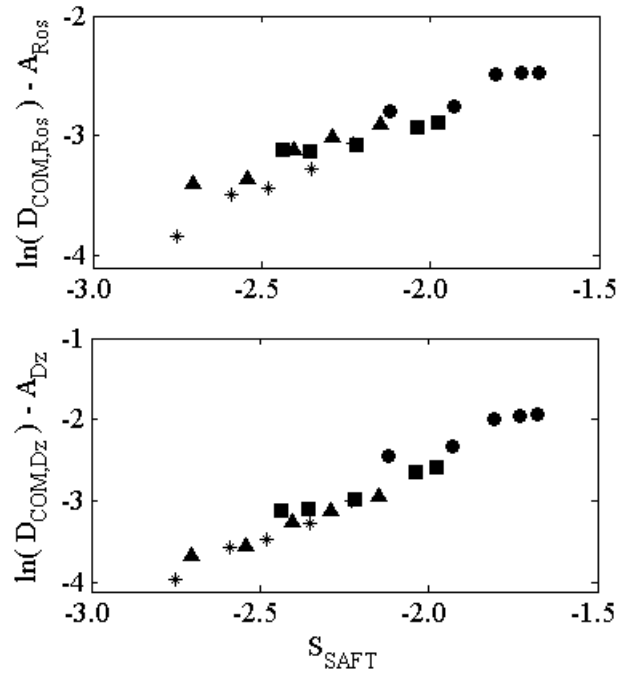


Figure S3. Correlation between both the Rosenfeld and the Dzugutov scaled diffusion coefficient reduced by the chain-length dependent terms  $A_{Ros}$  and  $A_{Dz}$  and the excess entropy predicted by SAFT.