Effect of the content and strength of hard segment on the

viscoelasticity of the polyurethane elastomer: Insight from molecular

dynamics simulation

Yimin Wang^{1, 2}, Ruibin Ma^{1,2}, Haoxiang Li^{1,2}, Shikai Hu^{1,2}, Yangyang Gao^{1,2*}, Li

Liu^{1,2*}, Xiuying Zhao^{1,2*}, Liqun Zhang^{1,2}

¹State Key Laboratory of Organic-Inorganic Composites, Beijing University of Chemical Technology, 100029 Beijing, People's Republic of China
²Key Laboratory of Beijing City on Preparation and Processing of Novel Polymer Materials, Beijing University of Chemical Technology, 100029 Beijing, People's Republic of China

^{*} Corresponding author: https://www.iui.buct.edu.cn or gov/anail.buct.edu.cn or gov/anail.buct.edu or <a hre=



Fig. S1 Schematic representation of the modelled hard-soft block PU chain containing 15 repeating units where the content of HS $\alpha_{\rm H}$ is 0.33.



Fig. S2 The glass transition temperature (T_g) of the pure HS polymer ($\alpha_{\rm H}$ =1.0) and the pure SS polymer ($\alpha_{\rm H}$ =0.0).



Fig. S3 The time-dependent shear stress σ_{xy} at shear strain amplitude (a) $\gamma_0 = 0.05$, (b) $\gamma_0 = 0.2$, (c) $\gamma_0 = 0.8$. The empty dots stand for the "batch averaged" shear stress while the continuous lines are sinusoidal fits to empty dots. (T^{*}=1.0, $\alpha_{\rm H} = 0.17$)



Fig. S4(a) The thermal energy exchange (ΔE_{ex}) contributed by (a) HS and (b) SS respectively with respect to the content of HS α_{H} for different shear strain amplitudes γ^{0} . (T^{*}=1.0)



Fig. S5 Schematic diagram of the energy difference (ΔE_{HH} , ΔE_{HS} , ΔE_{SS}) between HS and HS, HS and SS or SS and SS during the sinusoidal shear process. (α_{H} =0.5)