Electronic Supplementary Material (ESI) for Soft Matter.

Understanding Conformational and Dynamical Evolution of Semiflexible Polymers in Shear Flow

Xiangxin Kong[1,2], Yingchun Han[1,2], Wenduo Chen*[,3], Fengchao Cui[1], Yunqi Li*[,1,2]

1 Key Laboratory of High-Performance Synthetic Rubber and Its Composite Materials, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, 5625 Renmin Street, Changchun, PR China, 130022

2 University of Science and Technology of China, Hefei, PR China, 230026

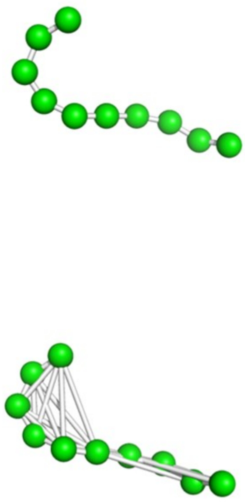
3 School of Materials, Sun Yat-sen University, No. 135, Xingang Xi Road, Guangzhou, P. R. China, 510275

* To whom correspondence should be addressed. E-mail: chenwd29@mail.sysu.edu.cn, yunqi@ciac.ac.cn. Phone: +86 (0)431 85262535

Supporting Information

① **Linear polymer (part)**

② **Distance selection**



③ **adjacency and contact matrix**

$$\mathbf{A}=\begin{pmatrix}0&1&1&1&0&0&0&0&0&0\\1&0&1&0&1&0&0&0&0&0\\1&1&0&1&1&1&0&0&0&0\\1&0&1&0&1&1&1&0&0&0\\0&1&1&1&0&1&1&1&1&1\\0&0&1&1&1&0&1&1&1&1\\0&0&0&1&1&1&0&1&1&1\\0&0&0&0&1&1&1&0&1&1\\0&0&0&0&1&1&1&1&0&1\\0&0&0&0&1&1&1&1&1&0\end{pmatrix}$$

④ **distance**

$$d_{ij}=\begin{pmatrix}0&1&1&1&2&2&2&3&3&3\\1&0&1&1&1&2&2&2&2&2\\1&1&0&1&1&1&2&2&2&2\\1&1&1&0&1&1&1&2&2&2\\2&1&1&1&0&1&1&1&1&1\\2&2&1&1&1&0&1&1&1&1\\2&2&2&1&1&1&0&1&1&1\\3&2&2&2&1&1&1&0&1&1\\3&2&2&2&1&1&1&1&0&1\\3&2&2&2&1&1&1&1&1&0\end{pmatrix}$$

Fig.S1. The introduction of the contact matrix and the shortest path for a linear polymer.

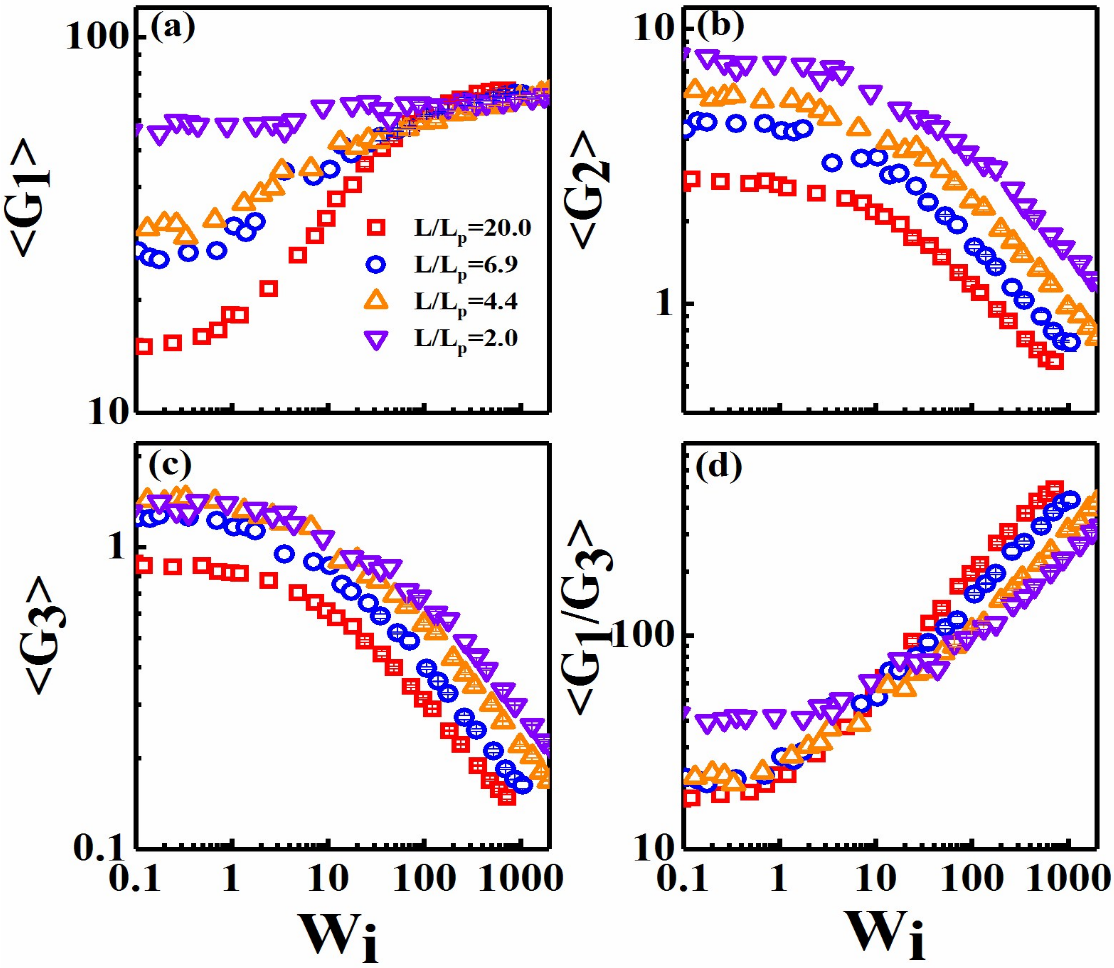


Fig.S2. (a) the largest eigenvalue G_1, (b) the intermediate eigenvalue G_2, (c) the smallest eigenvalue G_3, and (d) the elongation ratio G_1/G_3 in the gyration tensor as a function of *Wi* for polymer chains with increased rigidities L/L_p =20.0, 6.9, 4.4, and 2.0 respectively.

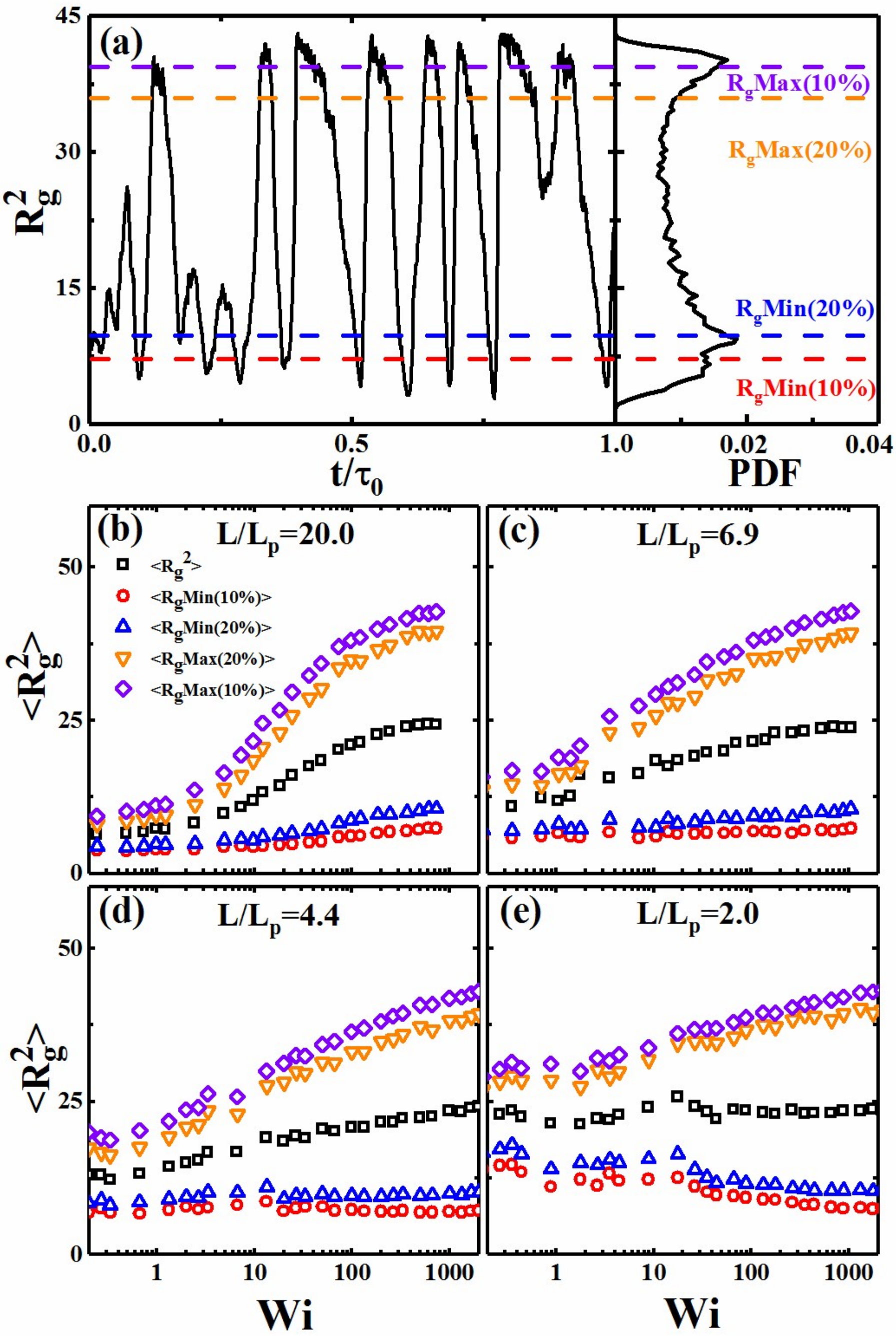


Fig.S3. A typical evolution of R_g^2 vs simulation time is shown in (a), (b-e) show the distribution of R_g^2, R_gMax and R_gMin of polymer chains with different rigidities as a function of Wi. The right profile in (a) is the normalized probability density function (PDF) of R_g^2. R_gMax (10%) and R_gMax (20%) are the cutoff values that cover largest 10% and 20% of the square radius of gyration R_g^2, accordingly, R_gMin (10%) and R_gMin (20%) are the cutoff values that cover the smallest side. Four sub-processes are defined according to R_gMax and R_gMin: the collapse process is between adjacent R_gMax and R_gMin, the stretching process is between adjacent R_gMin and R_gMax, the align & flip process represents the motions between two neighboring R_gMax, and the tumble represents the motions between two neighboring R_gMin.

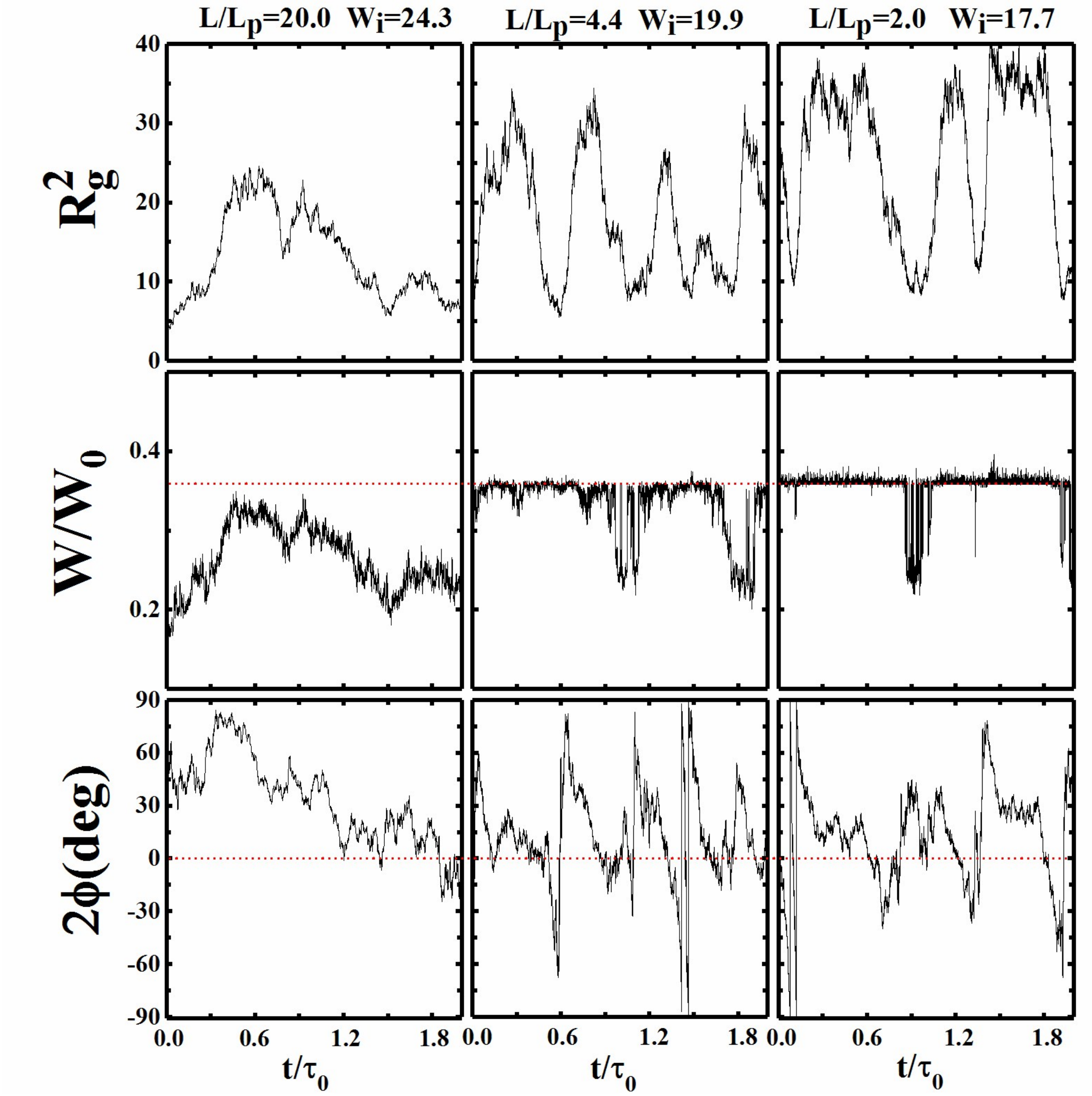


Fig.S4. The evolution of the square radius of gyration $R_g{}^2$, the normalized Wiener index W/W_0, and the orientation angle ϕ for polymer chains with different rigidities in intermediate shear flow.

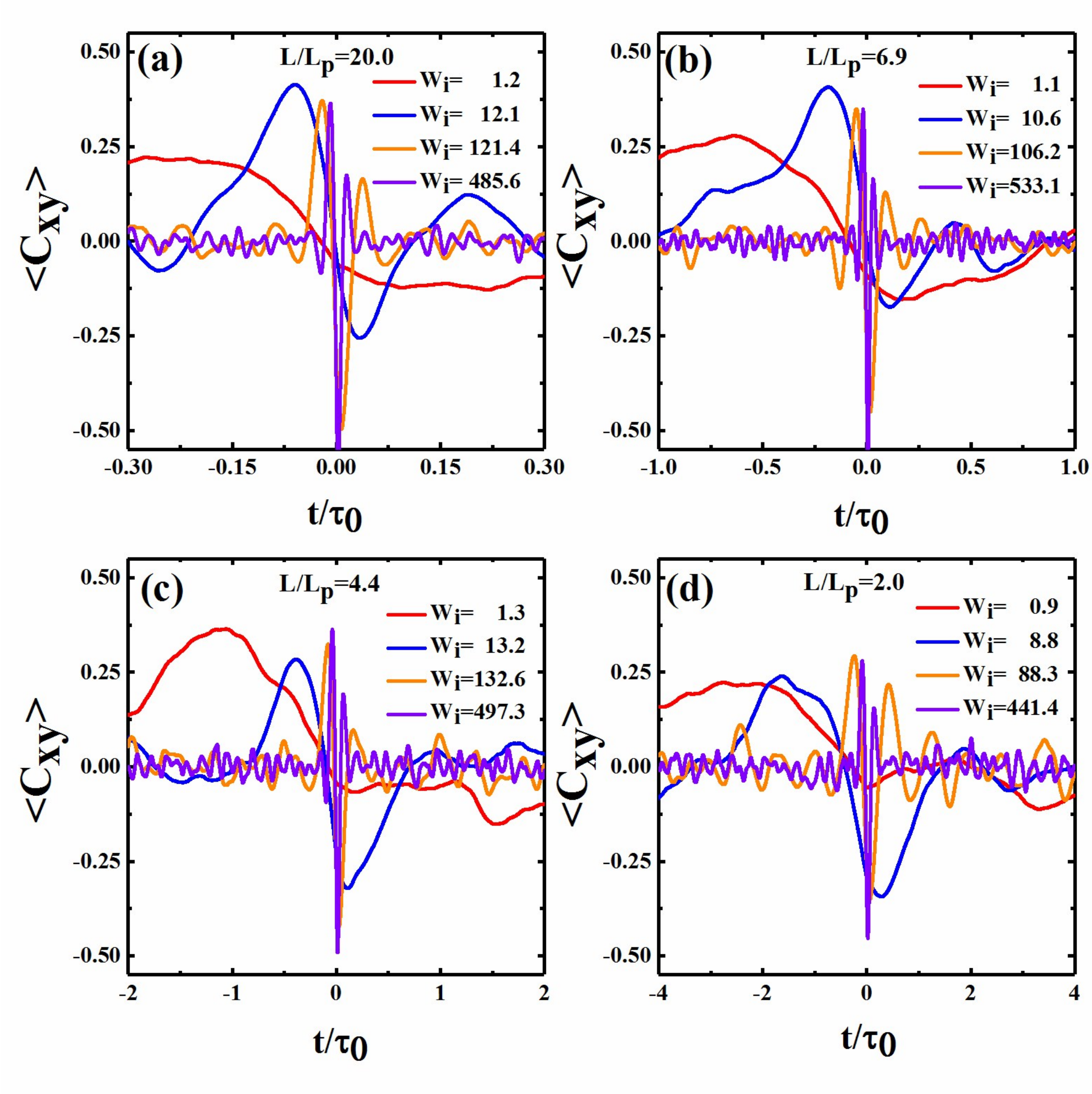


Fig.S5. Cross-correlation functions C_{xy} against reduced time scale for polymer chains at different Weissenberg numbers.

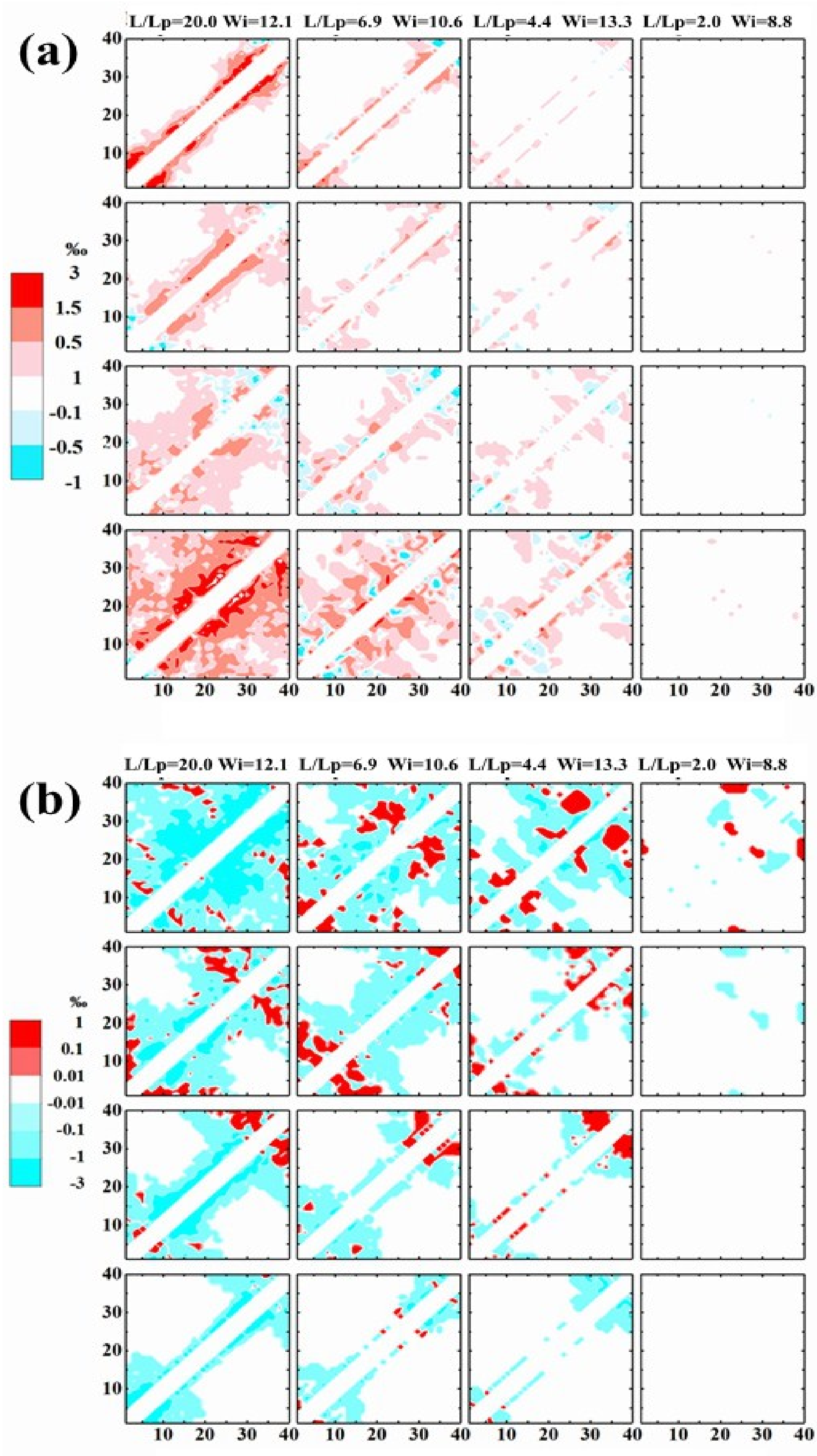


Fig.S6. The differential contact maps for (a) the collapse and (b) the stretching processes of polymer chains in intermediate shear flows.

SUPPLEMENTAL MATERIAL

See supplementary material for videos of flexible and semiflexible polymer chains in shear flow: Video 1, L/Lp=20.0, Wi=12.1; Video 2, L/Lp=4.4, Wi=13.3; Video 3, L/Lp=20.0, Wi=121.4; Video 4, L/Lp=4.4, Wi=132.6.