

## Supporting Information

### Cholesteric Ordering Predicted using a Coarse-grained Polymeric Model with Helical Interaction

Liang Wu and Huai Sun\*

School of Chemistry and Chemical Engineering and Key Laboratory of Scientific and Engineering Computing of Ministry of Education, Shanghai Jiao Tong University, 200240, Shanghai, China

Table 1 Equation of state for FCh molecules of chain length  $N_b = 10$ , chain flexibility  $K_{angle} = 100$ , internal chirality  $\phi_0 = 30^\circ$ . The isotropic phase is denoted by Iso and cholesteric phase by Chole.

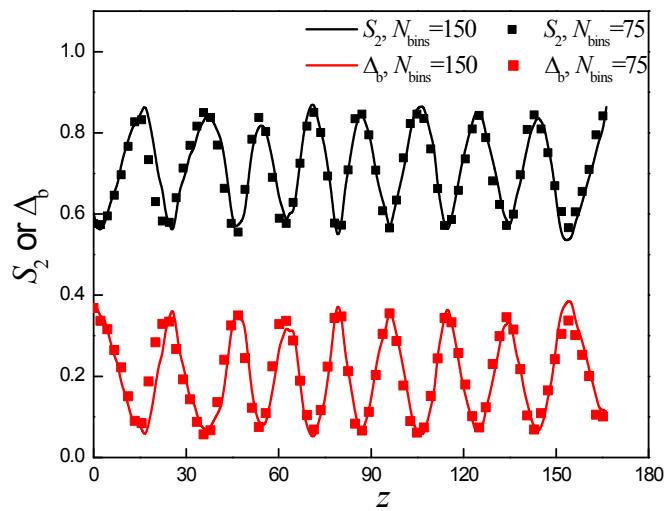
$\rho^*$	$P_z^*$	$S_2$	Phase
0.00878±0.0001	0.01	0.0120±0.001	Iso
0.01861±0.0002	0.03	0.0158±0.001	Iso
0.02458±0.0002	0.05	0.0211±0.001	Iso
0.02937±0.0003	0.07	0.0304±0.002	Iso
0.03151±0.0003	0.08	0.0312±0.002	Iso
0.03393±0.0003	0.09	0.0495±0.003	Iso
0.03857±0.0004	0.10	0.2182±0.003	Chole
0.03993±0.0004	0.11	0.2299±0.005	Chole
0.04143±0.0004	0.12	0.2419±0.005	Chole
0.04476±0.0004	0.15	0.2462±0.007	Chole
0.04822±0.0005	0.18	0.2601±0.007	Chole
0.04979±0.0005	0.20	0.2546±0.015	Chole

Table 2 Equation of state for FCh molecules of chain length  $N_b = 10$ , chain flexibility  $K_{angle} = 75$ , internal chirality  $\phi_0 = 30^\circ$ . The isotropic phase is denoted by Iso and cholesteric phase by Chole.

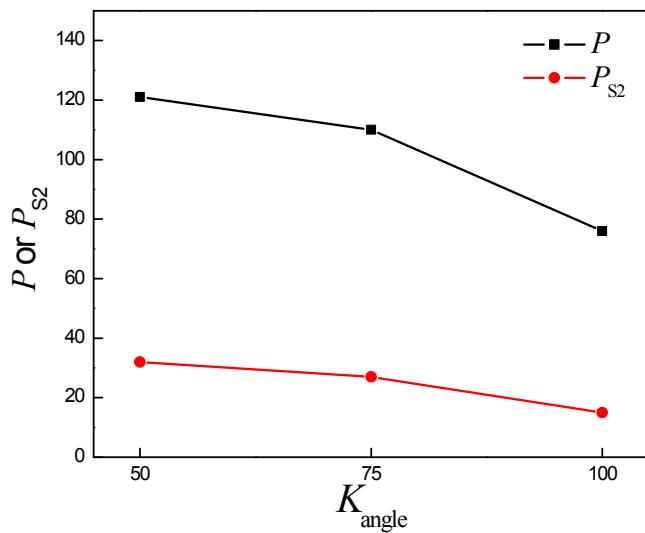
$\rho^*$	$P_z^*$	$S_2$	Phase
0.00878±0.0001	0.01	0.01273±0.001	Iso
0.01443±0.0001	0.02	0.01405±0.001	Iso
0.0185±0.0002	0.03	0.01501±0.002	Iso
0.02174±0.0002	0.04	0.01742±0.002	Iso
0.02447±0.0002	0.05	0.02046±0.002	Iso
0.02676±0.0003	0.06	0.02121±0.004	Iso
0.02895±0.0003	0.07	0.02318±0.004	Iso
0.03099±0.0003	0.08	0.03411±0.004	Iso
0.03319±0.0004	0.09	0.03556±0.005	Iso
0.03861±0.0004	0.10	0.19363±0.005	Iso
0.04086±0.0004	0.12	0.24354±0.005	Chole
0.04373±0.0005	0.14	0.24977±0.005	Chole
0.04618±0.0005	0.16	0.26271±0.008	Chole
0.04735±0.0005	0.18	0.26605±0.009	Chole
0.0488±0.0005	0.20	0.26952±0.012	Chole

Table 3. Equation of state for FCh molecules of chain length  $N_b = 10$ , chain flexibility  $K_{angle} = 50$ , internal chirality  $\phi_0 = 30^\circ$ . The isotropic phase is denoted by Iso and cholesteric phase by Chole.

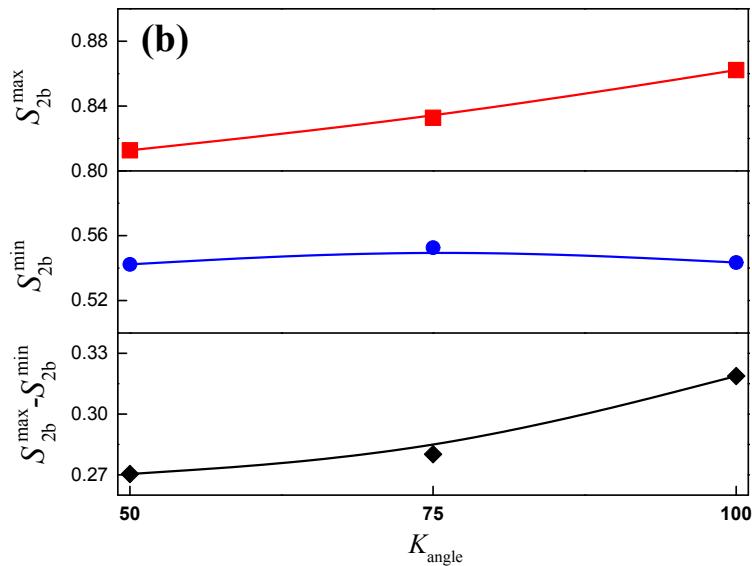
$\rho^*$	$P_z^*$	$S_2$	Phase
0.00872±0.0001	0.01	0.01179±0.001	Iso
0.01431±0.0001	0.02	0.01325±0.002	Iso
0.01827±0.0002	0.03	0.01419±0.002	Iso
0.02147±0.0002	0.04	0.01732±0.004	Iso
0.02639±0.0003	0.06	0.02098±0.004	Iso
0.02843±0.0003	0.07	0.0206±0.006	Iso
0.03032±0.0003	0.08	0.03219±0.006	Iso
0.03209±0.0003	0.09	0.02622±0.007	Iso
0.03393±0.0003	0.10	0.05701±0.007	Iso
0.0366±0.0004	0.11	0.07308±0.007	Iso
0.03917±0.0004	0.12	0.22583±0.009	Chole
0.04218±0.0004	0.14	0.25736±0.010	Chole
0.04439±0.0004	0.16	0.25583±0.011	Chole
0.0468±0.0005	0.18	0.26872±0.011	Chole
0.04788±0.0005	0.20	0.26996±0.015	Chole



**Figure S1.** Profiles of local nematic order parameter  $S_2(z)$  and local biaxiality parameter  $\Delta_b(z)$  calculated using different numbers of bins: curves ( $N_{bin} = 150$ ) and squares ( $N_{bin} = 75$ ).



**Figure S2.** Average cholesteric pitch  $P$  and periodicity of  $S_2(z)$  profile as functions of molecular flexibility parameter  $K_{angle}$  describing the angle bending of FCh backbone.



**Figure S3.** Minimum ( $S_{2b}^{\text{min}}$ ) and maximum ( $S_{2b}^{\text{max}}$ ) in  $S_2(z)$  profile at  $P_z^* = 0.18$  with molecular flexibilities  $K_{\text{angle}} = 100, 75, 50$ , and the amplitude ( $S_{2b}^{\text{max}} - S_{2b}^{\text{min}}$ ).