Conformational behavior of a semiflexible dipolar chain with a variable relative size of charged groups via molecular dynamics simulations.


Supporting information.

Figure S1. Radius of gyration $R_{gyr}$ (left) and persistence length $l_p$ (right) as functions of rigidity $k$ in the case of the ideal chain (gauss) and for uncharged chains in good solvent with different dipole length $d = 1.0$ and 1.5.
Figure S2. Distance map for backbone units with dipole length $d = 1$ for different $k = 8, 11, 12, 16$ at $\lambda = 10$. 
Figure S3. Number of turns of the torus as function of $\lambda$ at different $k$ and $d = 1$.

Figure S4. The average cosine between dipoles as function of number along chain for different $k$ at $\lambda = 10$ and $d = 1$. 
Figure S5. The average cosine between dipoles neighboring along the chain along as function of distance in space for different $k$ at $\lambda = 10$ and $d = 1$. 
Figure S6. Radial distribution functions of backbone beads relative to each other, $g_{mm}$, as well as relative to side beads, $g_{mc}$, for different $\lambda$ and $k$ at $d = 1$
Figure S7. Radial distribution functions of backbone beads relative to the center of mass of the chain for different $\lambda$ and $k$ at $d = 1$.

Figure S8. Snapshots of dipolar chain of rigidity $7 \leq k \leq 14$ at $\lambda = 10$, $N = 32$. There are metastable states such as circle, hairpin and extended chain.
Figure S9. Snapshots of dipolar chain at \( \lambda = 20 \), \( N = 32 \). There are loose globule \((k = 15)\), knots with trefoil knot \((k = 26)\), hairpin with short-living torus \((k = 34)\) and rod \((k = 40)\).

Figure S10. Dynamic exchange between toroidal structure, hairpin and extended chain in a typical run, as seen in the trace of radius of gyration as a function of time for different rigidity at \( \lambda = 10 \). Top: \( N = 32 \) and \( k = 7, 10, 14 \). Bottom: \( N = 64 \) and \( k = 7, 14, 19 \).
Figure S11. Snapshots of dipolar chain of rigidity $k = 7, 14, 19$ at $\lambda = 10, N = 64$.

Figure S12. Radius of gyration $R_{gyr}$ as function of rigidity $k$ at $\lambda = 20, N = 64$.

Figure S13. Snapshots of dipolar chain of rigidity $k = 14, 19$ at $\lambda = 20, N = 64$. There are globule and torus.
Figure S14. Radius of gyration $R_{\text{gyr}}$ as function of rigidity $k$ at $\lambda = 10$, $N = 128$.

Figure S15. Snapshots of 128-chain for $11 \leq k \leq 20$, $\lambda = 10$, $d = 1$. 
Figure S16. Radial distribution function (density) of backbone units from the center of mass of the chain for different \( k \) at \( \lambda = 10 \). From top to bottom: \( d = 0.6, 0.7, 1.1, 1.2 \).