Supplementary Material

Atomistic Insights into Liquid Crystals of Board-Like Molecules via Molecular Dynamics Simulation

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1. Nematic order parameter

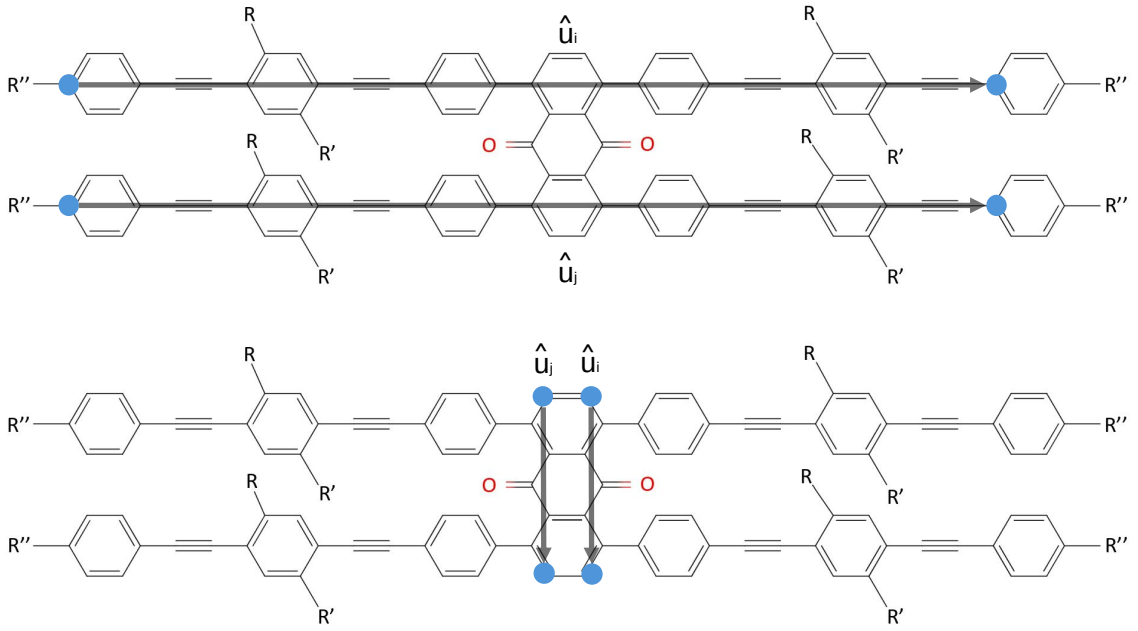

Figure S.1: Definition of the unit vectors $\hat{u}_i$ and $\hat{u}_j$ determining the orientation of a generic mesogen and applied to compute the nematic order parameter S_{2L} (top) and S_{2W} (bottom). Initial and terminal points of these vectors are represented by a pair of reference carbon atoms indicated by light-blue circles.

The nematic order parameters are the eigenvalues of the following tensor

$$\mathbf{Q}_{\alpha\beta} = \frac{1}{2N}\sum_{j=1}^{N}\left(3\hat{\mathbf{u}}_{j\alpha}\hat{\mathbf{u}}_{j\beta} - \mathbf{I}\right) \tag{1}$$

where the unit vectors $\hat{\mathbf{u}}_{j\alpha}$ quantify the orientation of molecule j, (α,β) are mutually orthogonal space dimensions (x, y, z), and $\mathbf{I}$ is the unit tensor. The unit vectors $\hat{\mathbf{u}}_{j\alpha}$ are obtained as the normalised distance between two reference C atoms belonging to the upper or lower arms of each molecule as shown in Fig. S.1. Although one of these two vectors is sufficient to determine molecular orientation, we have used two per molecule to improve statistics. On average, the order parameters obtained from each of them are identical.

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2. Snapshots of nematic-like clusters

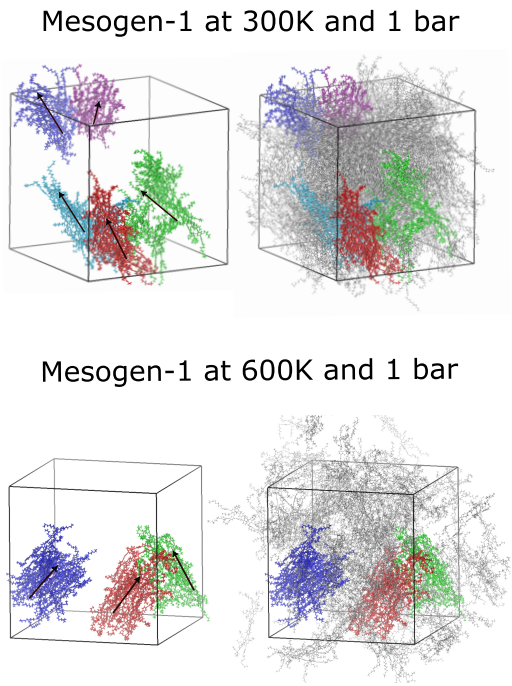

Figure S.2: Nematic-like clusters observed in weakly-ordered phases of mes-1 at 300 K (top frame) and 600 K (bottom frame), both at 1 bar. The left snapshots exclude misaligned molecules, while the right snapshots include them. Different colours represent molecules belonging to distinct nematic domains, with grey indicating molecules not part of any cluster. Black arrows indicate the approximate orientation of the molecules in each cluster.

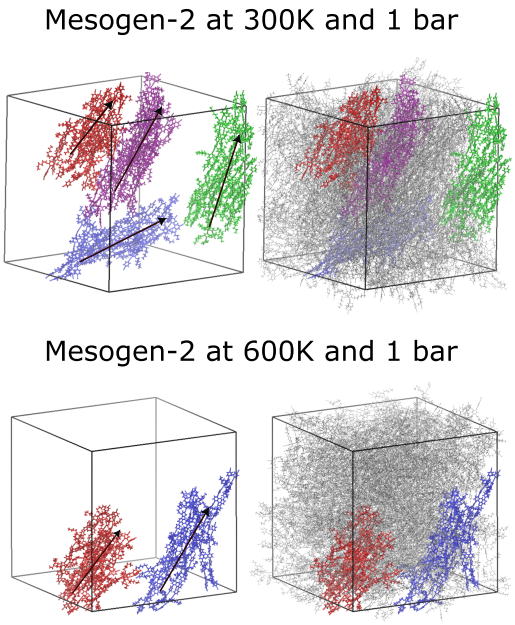

Figure S.3: Nematic-like clusters observed in weakly-ordered phases of mes-2 at 300 K (top frame) and 600 K (bottom frame), both at 1 bar. The left snapshots exclude misaligned molecules, while the right snapshots include them. Different colours represent molecules belonging to distinct nematic domains, with grey indicating molecules not part of any cluster. Black arrows indicate the approximate orientation of the molecules in each cluster.

3. Radial distribution functions of mes-1 and mes-2

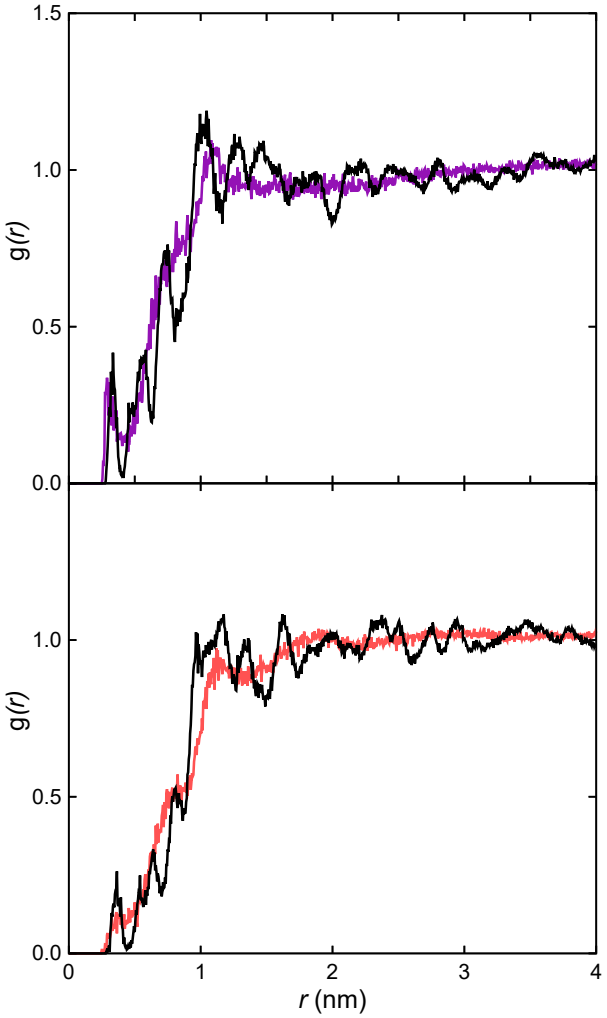

Figure S.4: Radial distribution function for mes-1 (top frame) and mes-2 (bottom frame) at 300 K (black line) and 600 K (colored) at 1 bar.

4. Mean-squared displacements of mes-1 and mes-2

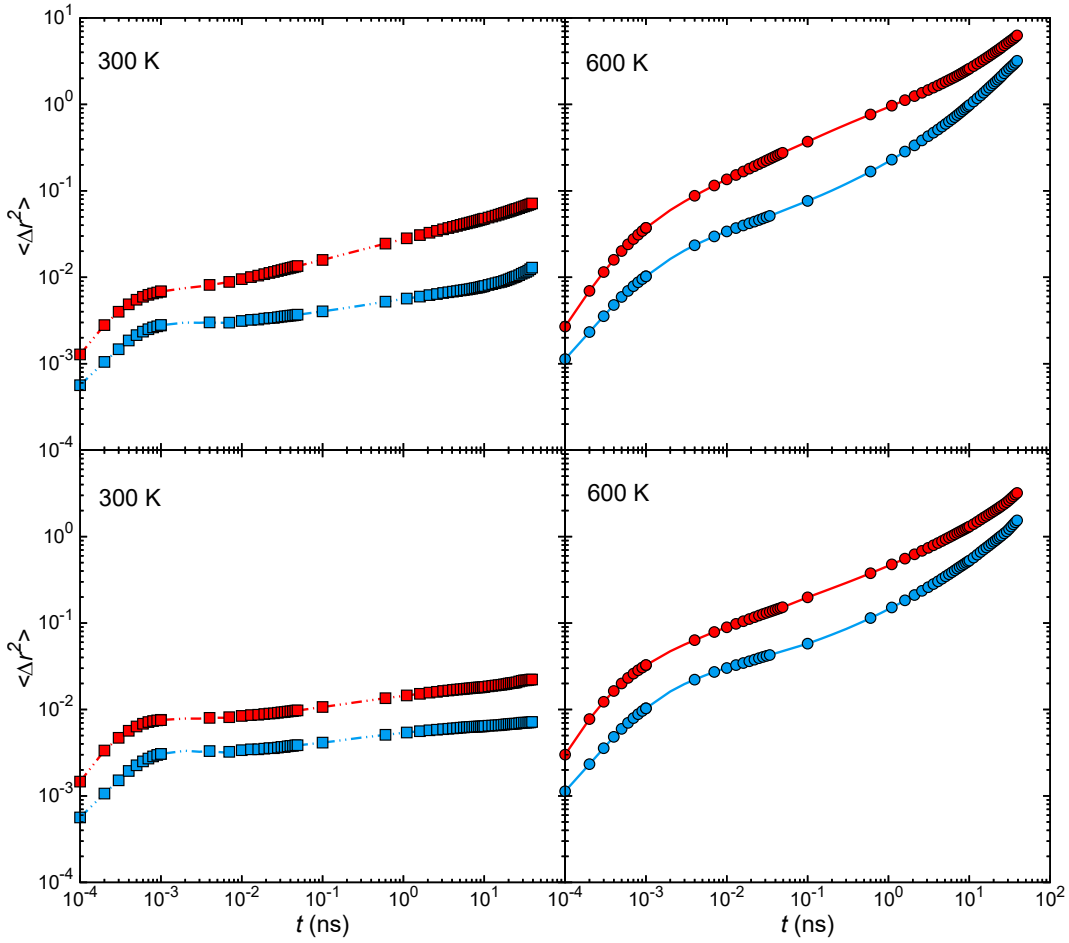

Figure S.5: Mean-squared displacement of mes-1 (top frames) and mes-2 (bottom frames) at 300 K (left frames) and 600 K (right frames) for the terminal (red symbols) and core group (blue symbols) at 1 bar. The solid and dot dashed lines are a guide for the eye.

5. Self-part of the van Hove functions of mes-1 and mes-2

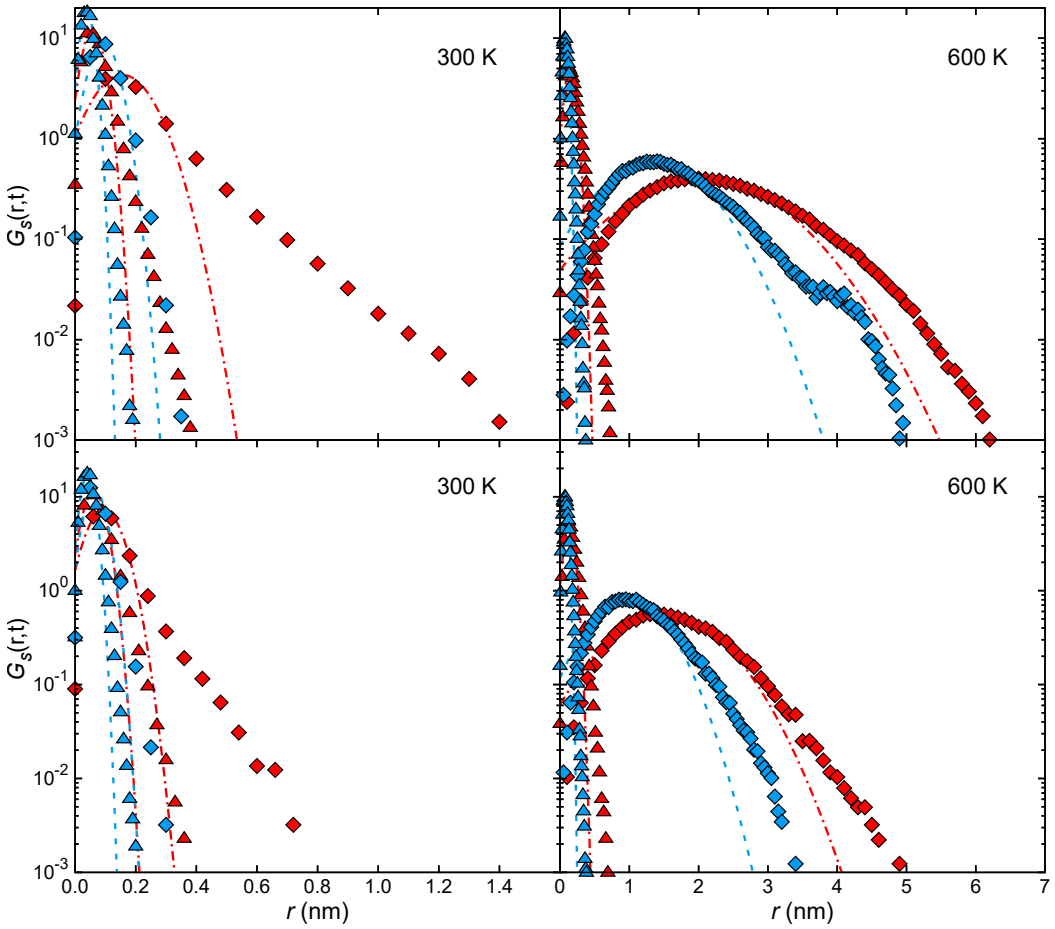

Figure S.6: Self-part of the van Hove correlation functions of mes-1 (top frames) and mes-2 (bottom frames) at 300 K (left frames) and 600 K (right frames). Red and blue symbols refer, respectively, to the mesogen terminal and core groups at $t = 10^{-3}$ ns (triangles) and $t = 40$ ns (rhombus). Blue dashed and red dash-dotted lines are Gaussian fits of the s-VHFs of core and terminal groups, respectively.