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Title	Parameterization of the Gay-Bern potential for nCB and molecular dynamics simulation of 5CB
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Purpose of this study	In most of mesogens, the tail plays an important role in determining their phase behavior. The purpose of this study is to examine the dependence of the phase behavior on the parameters of the coarse-grained potential, and to analyze the effect of the tail.
System (Material)	5CB(4-n-pentyl-4'-cyanobiphenyl)
Program (including analysis)	COGNAC v1.2 hand-made analysis tool(order parameter, RDF)
Method & Some important input parameters	(Method) Molecular dynamics simulation using the model, where an 5CB molecule is divided into a rigid part and a flexible part. (Input) Number of molecules, NPT ensemble, Gay-Berne potential, Lennard-Jones potential, temperature, pressure
Advance & Problem	Advance: We have carried out MD simulations of 5CB to examine the parameter dependency of the structure, the density of the ordered state and the transition temperature. We found that if the length of the rigid core is kept constant, the isotoropic phase becomes favored with increasing the aspect ratio of the core. This can be explained as the effect of the thickness of the tail part. Problem: We would require to include the terminal dipole.
Reference	[Manuscript] : Accepted Prog. Theoret. Phys. Suppl., 138, 396 (2000). Mol. Cryst. Liquid Cryst., in press. [Presentation at conferences (Meetings)] The 5th International Conference on Computational Physics (ICCP5) (1999) Japan Liquid Crystal Society conference(1999,2000) The 18th International Liquid Crystal Conference (ILCC2000) (2000)
KeyWord (in English)	molecular dynamics (MD) simulation , Gay-Berne (GB) potential, Lennard-Jones (LJ) potential, OPLS potential, liquid crystal, nematic, nCB(4-n-alkyl-4'-cyanobiphenyl)

Results (Remarks)

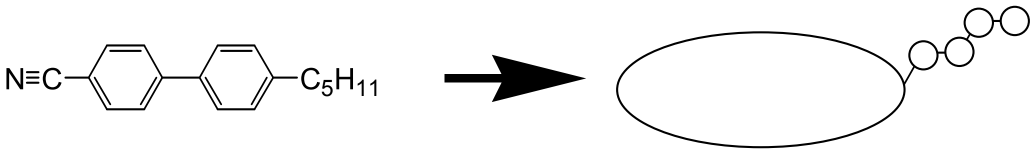

Fig.1 GB-LJ hybrid model for 5CB molecule.

(a) (b)

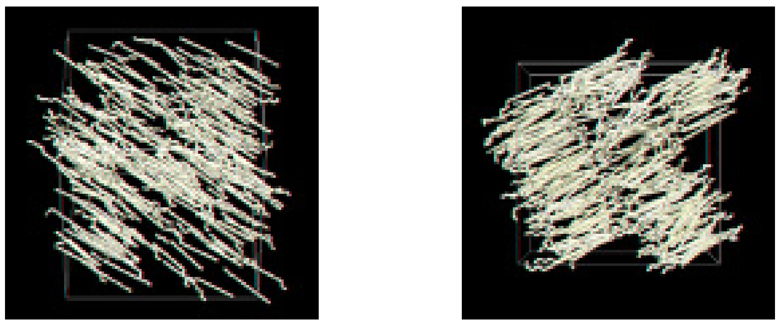

Fig.2 Snap shot of the liquid crystal phase obtained using the GB potential represented by (a) length-breadth ratio of 3.4and (b) 4.0 for 5CB molecule.

Appendix

Gay-Berne potential

$$U(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\mathbf{r}_{ij}) = 4\varepsilon(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij})\left[\left(\frac{\sigma_0}{r_{ij}-\sigma(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij})+\sigma_0}\right)^{12}-\left(\frac{\sigma_0}{r_{ij}-\sigma(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij})+\sigma_0}\right)^{6}\right]$$

$$\sigma(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij}) = \sigma_0\left[1-\frac{\chi}{2}\left\{\frac{\left((\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_i)+(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_j)\right)^2}{1+\chi(\hat{\mathbf{u}}_i\cdot\hat{\mathbf{u}}_j)}+\frac{\left((\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_i)-(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_j)\right)^2}{1-\chi(\hat{\mathbf{u}}_i\cdot\hat{\mathbf{u}}_j)}\right\}\right]^{-1/2}$$

$$\varepsilon(\hat{\mathbf{u}}_i,\hat{\mathbf{u}}_j,\hat{\mathbf{r}}_{ij}) = \varepsilon_0\left[1-\chi^2(\hat{\mathbf{u}}_i\cdot\hat{\mathbf{u}}_j)^2\right]^{-\nu/2}\left[1-\frac{\chi'}{2}\left\{\frac{\left((\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_i)+(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_j)\right)^2}{1+\chi'(\hat{\mathbf{u}}_i\cdot\hat{\mathbf{u}}_j)}+\frac{\left((\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_i)-(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{u}}_j)\right)^2}{1-\chi'(\hat{\mathbf{u}}_i\cdot\hat{\mathbf{u}}_j)}\right\}\right]^{\mu}$$

$$\chi = \left[\frac{(\sigma_e/\sigma_s)^2-1}{(\sigma_e/\sigma_s)^2+1}\right] \qquad \chi' = \left[\frac{(\varepsilon_s/\varepsilon_e)^{1/\mu}-1}{(\varepsilon_s/\varepsilon_e)^{1/\mu}+1}\right]$$