Supplemental Material

Impurity-induced nematic-isotropic transition of liquid crystals

Pritam Kumar Jana[a,f] Julien Lam,[b] Rahul Mangal[c], Mikko J Alava,[a] Nagma Parveen*[d] and Lasse Laurson*[e]*

[a]*COMP Centre of Excellence, Department of Applied Physics, Aalto University, Espoo, Finland*

[b]*CEMES, CNRS and Universite de Toulouse, 29 rue Jeanne Marvig, 31055 Toulouse Cedex, France*

[c]*Department of Chemical Engineering , Indian Institute of Technology Kanpur, Kalyanpur, Kanpur, India*

[d]*Department of Chemistry, Indian Institute of Technology Kanpur, Kalyanpur, Kanpur, India*

[e]*Computational Physics Laboratory, Faculty of Engineering and Natural Sciences, Tampere University, Finland*

[f]*Institute for Theoretical Physics, Department of Physics, University of Goettingen, Germany*

Force field parameters for 6CB

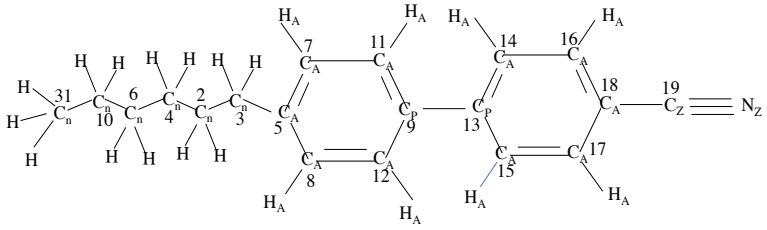

Figure S1. Structural details of 6CB molecule. All digits stand for the identity of the atoms. C_A and H_A are aromatic carbon and aromatic hydrogen. C_P is the ring joining carbon atom. C_n and H represent aliphatic carbon and hydrogen. C_z and N_z are the carbon and nitrogen from the cyano group. When we define the atoms using digits as suffix we consider C_A, C_P, C_n, C_Z≡C or H_A≡H.

Bond	k_l(eV Å^{-2})	l_0(Å)
C_A-H_A	33.96	1.08
C_A-C_A	44.32	1.38
C_A-C_P	44.32	1.38
C_P-C_P	27.28	1.47
C_A-C_Z	31.52	1.31
C_Z-N_Z	115.11	1.17
C_A-C_n	24.47	1.50
C_n-C_n	22.97	1.51
C_n-HC	31.65	1.09

Table S1. Bond stretching force constants ($\boldsymbol{k_l}$) and equilibrium bond lengths ($\boldsymbol{l_0}$)

Angle	k_θ($\times 10^{-5}$ eV/deg^2)	θ_0(degree)
C_A-C_A-H_A	98.46	120
C_A-C_A-C_A	84.94	120
C_A-C_P-C_P	95.32	120
C_A-C_A-C_Z	134.38	120
C_A-C_Z-N_Z	71.10	180
C_n-C_n-C_n	244.76	113
C_n-C_n-HC	116.98	112
HC-C_n-HC	147.25	107
C_n-C_A-C_A	185.53	120
C_A-C_n-HC	92.466	109.5
C_A-C_n-C_n	166.44	114

Table S2. Bond angle bending force constants ($\boldsymbol{k_\theta}$) and equilibrium bond angle ($\boldsymbol{\theta_0}$) for 6CB used in the simulations.

Torsion	$k_1(\times 10^{-2}$ eV)	$k_2(\times 10^{-2}$ eV)	$k_3(\times 10^{-2}$ eV)	$k_4(\times 10^{-2}$ eV)
C_A-C_A-C_A-C_A	0.0	41.240011	0.0	0.0
HC-C_n-C_n-C_n	0.0	0.0	0.16	0.0
HC-C_n-C_n-HC	0.0	0.0	0.14	0.0
C_A-C_P-C_P-C_A	0.0	7.9	0.0	1.76
C_A-C_n-C_n-C_n	3.04000011	0.03000016	-0.1400002	0.54998707
C_n-C_n-C_n-C_n	8.47	0.32	0.12	-1.63
C_A-C_A-C_n-C_n	0.0	3.59	0.0	-0.29

Table S3. Torsional force constants ($\boldsymbol{k_1, k_2, k_3, k_4}$) for 6CB used in simulations.

Atom	Charge (e)
Nz	-0.43
C_{19}	0.395
C_{18}	0.035
$C_{14,15,16,17,11,12,7,8}$	-0.122
$C_{13,9,5}$	0
$C_{2,3,4,6,10}$	-0.12
C_{31}	-0.18
H_A	0.122
H	0.06

Table S4. Partial charges for all atoms of 6CB molecule used in simulations.

Atom	ϵ (eV)	σ (Å)
Nz	0.00737	3.200
C_{19}	0.00651	3.650
C_{18}	0.00304	3.550
$C_{14,15,16,17,11,12,7,8}$	0.00304	3.550
$C_{13,9,5}$	0.00304	3.550
$C_{2,3,4,6,10}$	0.00286	3.500
C_{31}	0.00286	3.500
H_A	0.001306	2.420
H	0.001306	2.500

Table S5. $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ for all atoms of 6CB molecule used in simulations.

Force field parameters for hexane

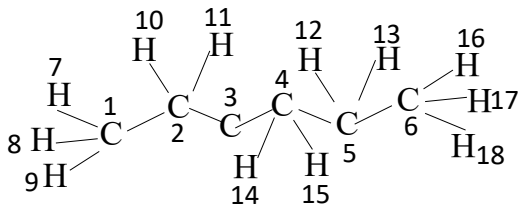

Figure S2. Chemical structure of hexane.

Bond	k_l(eV Å^{-2})	l_0(Å)
C-C	23.2432	1.529
C-H	29.4876	1.090

Table S6. Bond stretching force constants ($\boldsymbol{k_l}$) and equilibrium bond lengths ($\boldsymbol{l_0}$).

Angle	k_θ($\times 10^{-5}$ eV/deg^2)	θ_0(degree)
C-C-C	154.1546915	112.7
C-C-H	99.07376966	110.7
H-C-H	87.18150558	107.8

Table S7. Bond angle bending force constants ($\boldsymbol{k_\theta}$) and equilibrium bond angle ($\boldsymbol{\theta_0}$) for hexane used in the simulations.

Torsion	k_1($\times 10^{-2}$ eV)	k_2 ($\times 10^{-2}$ eV)	k_3 ($\times 10^{-2}$ eV)	k_4($\times 10^{-2}$ eV)
C-C-C-C	7.54536	-0.68081661	1.209859	0.00
H-C-C-H	0.000	0.000	1.378979	0.000
H-C-C-C	0.000	0.000	1.587127	0.000

Table S8. Torsional force constants ($\boldsymbol{k_1, k_2, k_3, k_4}$) for hexane used in simulations.

Atom	Charge (e)
$C_{1,6}$	-0.18
$C_{2,3,4,5}$	-0.12
H	0.06

Table S9. Partial charges for all atoms of hexane molecule used in simulations.

Atom	ϵ (eV)	σ (Å)
C	0.002862032	3.50
H	0.00130092	2.50

Table S10. $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ for all atoms of hexane molecule used in simulations.

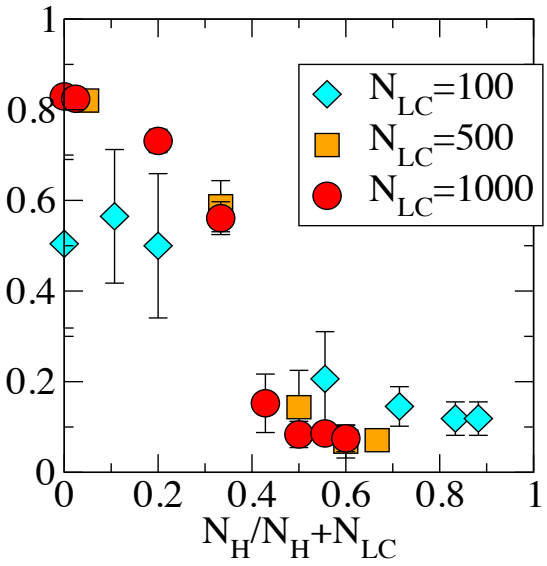

Figure S3. Order parameters of liquid crystals as a function of hexane concentration for different number of liquid crystals.

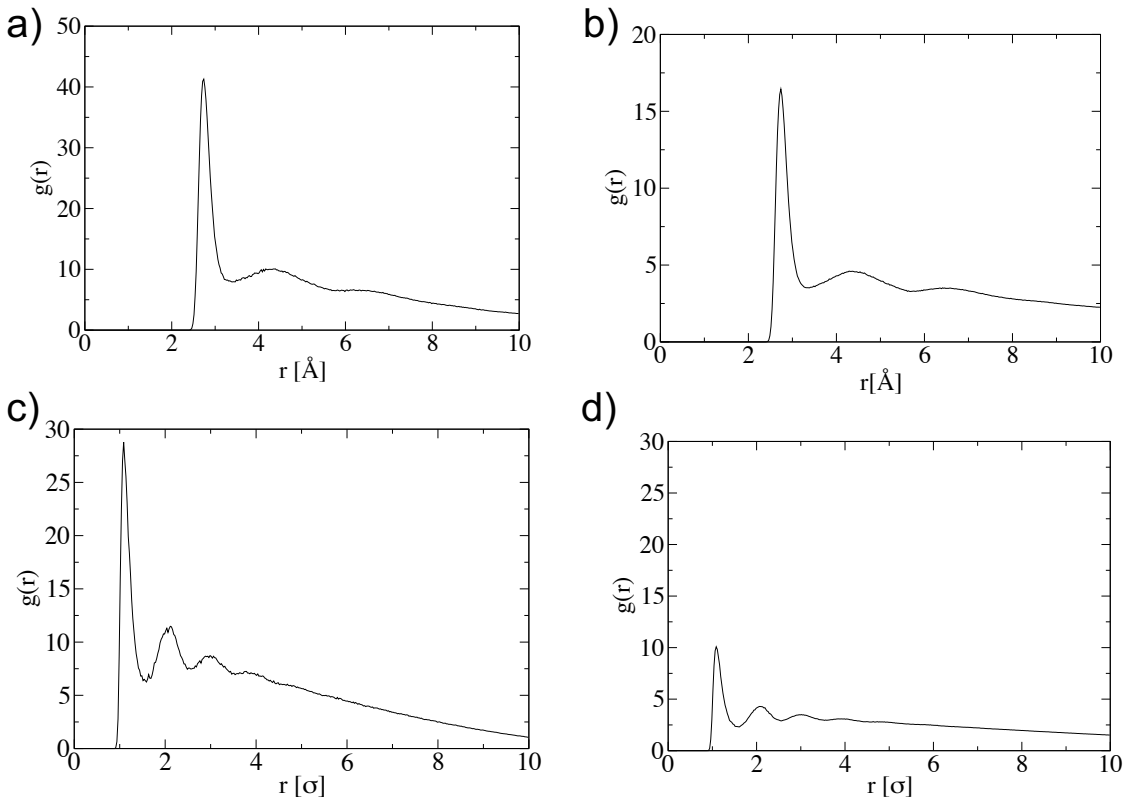

Figure S4. Radial distribution function of water in 6CB calculated from AA simulations for a) 72 water molecules in 72 6CB and b) 216 water molecules in 72 6CB. Radial distribution function of water in 6CB calculated from CG simulations for c) 1000 water molecules in 1000 6CB and d) 4000 water molecules in 1000 6CB.

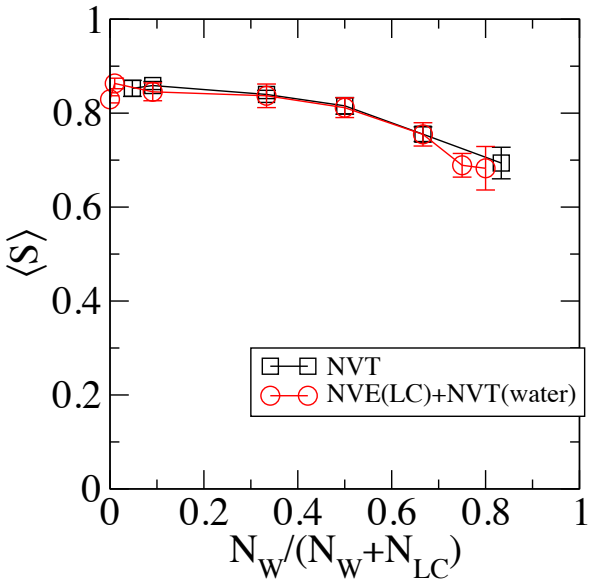

Figure S5. Comparison of order parameter of LC+water systems (N_{LC} = 1000) calculated from CG simulations using pure NVT and hybrid NVE+NVT.

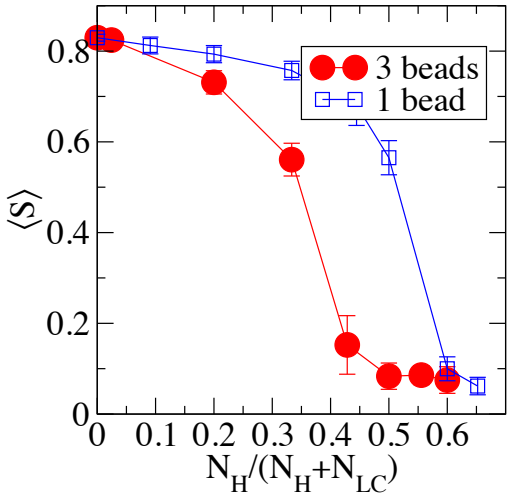

Figure S6. Comparison of order parameter of LC+hexane system (N_{LC} = 1000) calculated from hybrid model in CG simulations using LC chain as 8 beads and hexane as either 3 beads or 1 bead, respectively.

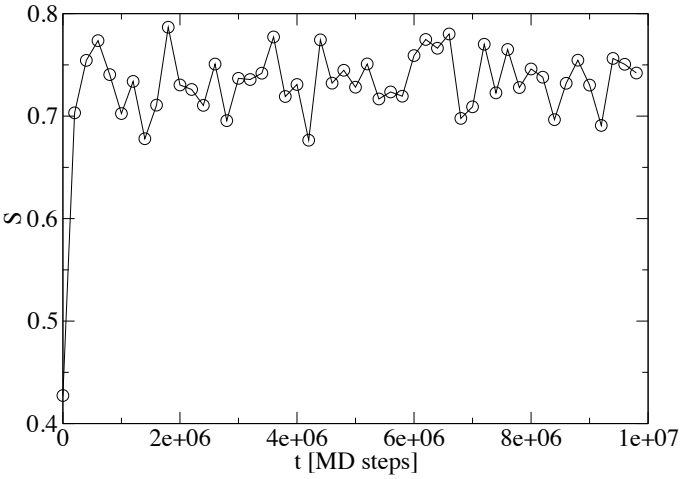

Figure S7. Time evolution of the order parameter, S of 6CB in presence of 250 hexane.

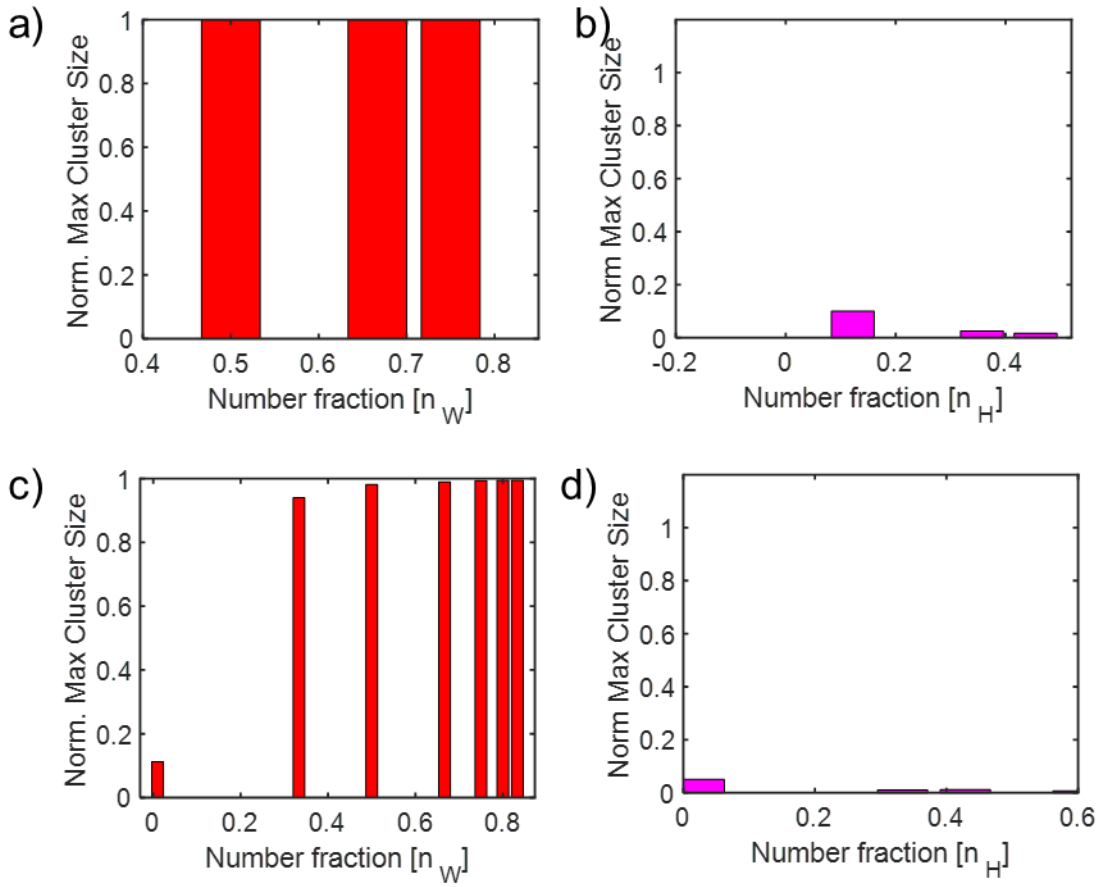

Figure S8. Maximum cluster size normalized with respect to total added impurity at the given number fraction of water**.**