Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Information

Spontaneously Chiral Cubic Liquid Crystal: Three Interpenetrating Networks with a Twist

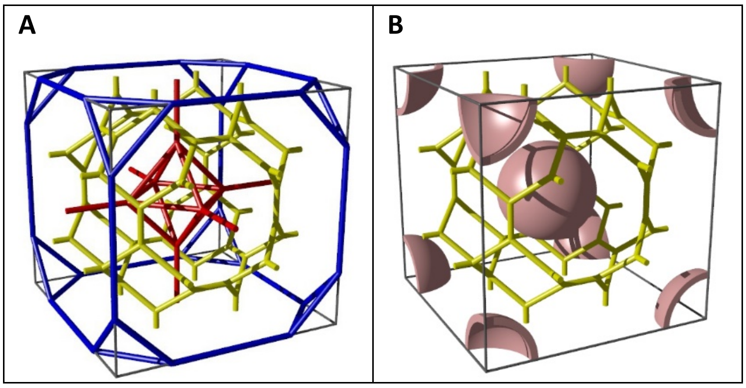
Xiangbing Zeng[1]* and Goran Ungar[1,2]

1. Department of Materials Science and Engineering, University of Sheffield, Sheffield S1 3JD, UK

2. State Key Laboratory for Mechanical Behaviour of Materials, Xi'an Jiaotong University, Xi'an, 710049 P. R. China

S1. Previous models of the chiral bicontinuous cubic phase

Figure S1. Two previous models of the chiral bicontinuous cubic phase, both with space group $Im\bar{3}m$. (A) Model with three interpenetrating networks: inner (red), middle (yellow) and outer (blue) (Ref. S1). (B) Model with one infinite network and vesicles. The network is more or less the same as the middle network of Model A, but the inner and outer networks of Model A are replaced with vesicles (pink) at the corners and the body centre of the unit cell (Ref. S2).



S2. Structural models

Figure S2. Different views of the inner network.

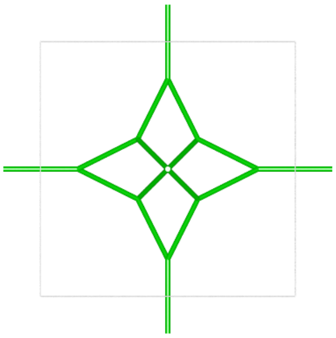
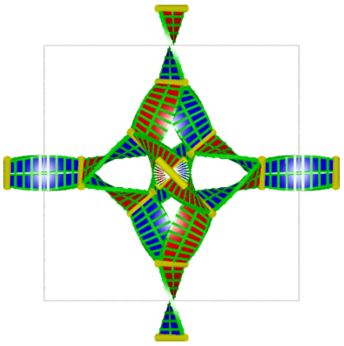
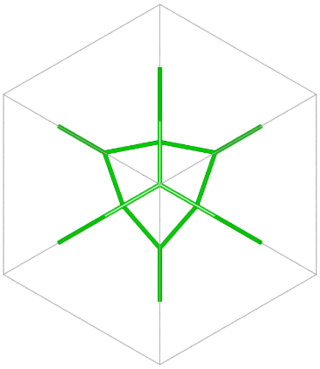
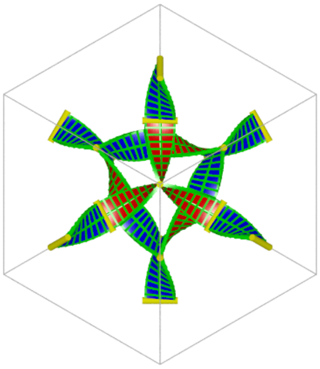
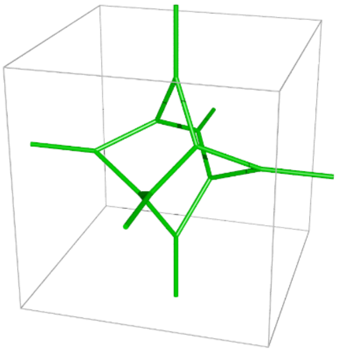
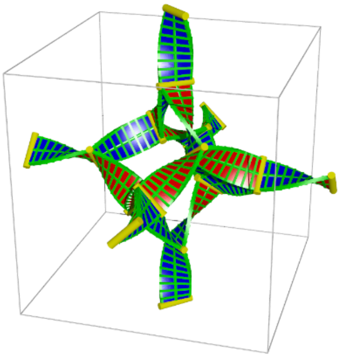
	Rods	Ribbons
View along (100)		
View along (111)		
Oblique view		

Figure S3. Different views of the inner and outer networks.

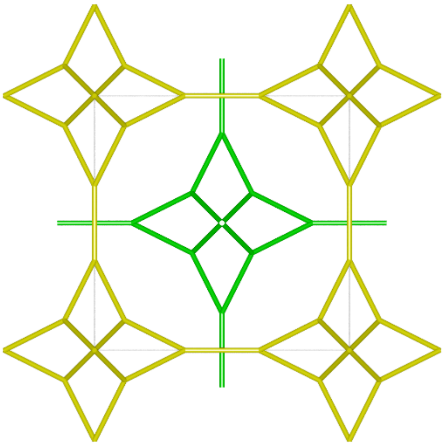
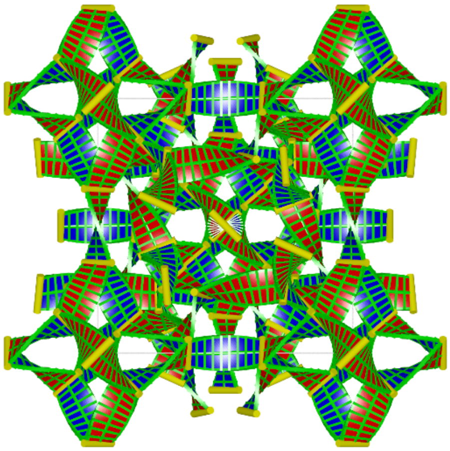
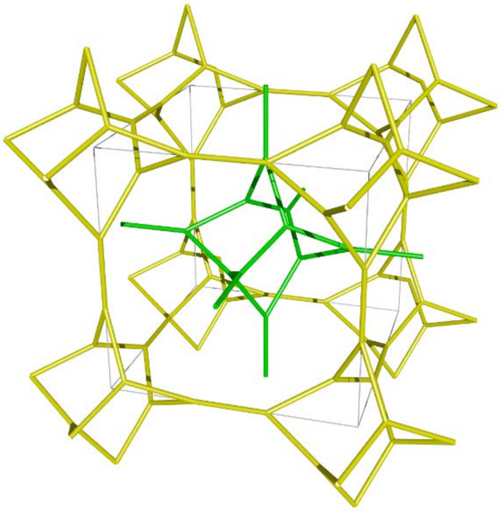
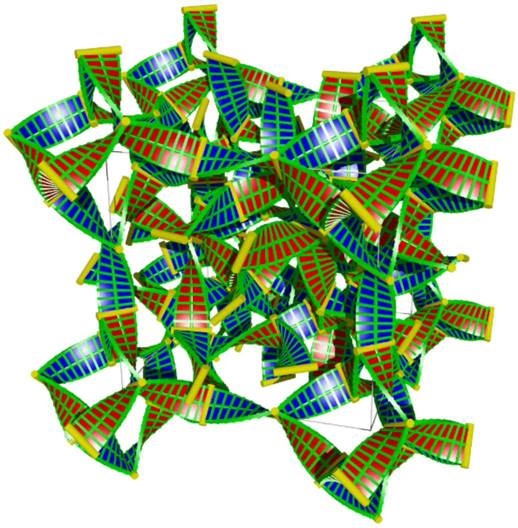
	Rods	Ribbons
View along (100)		
Oblique view		

Figure S4. Different views of the middle network

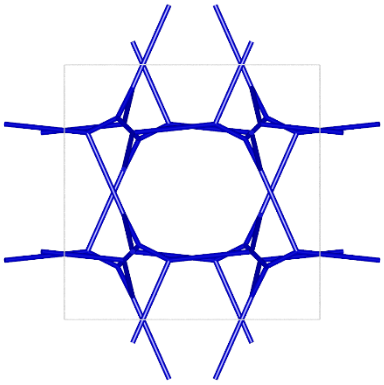
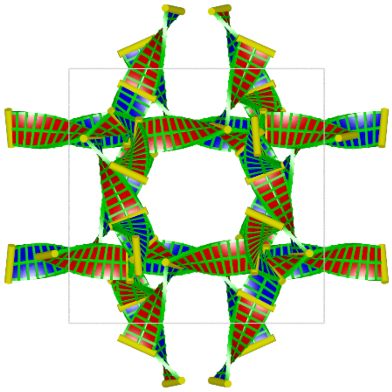
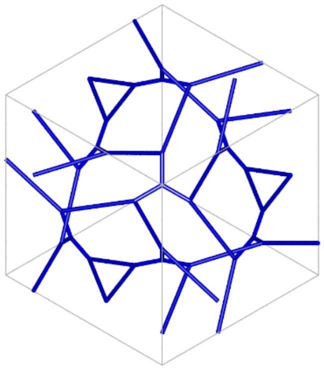
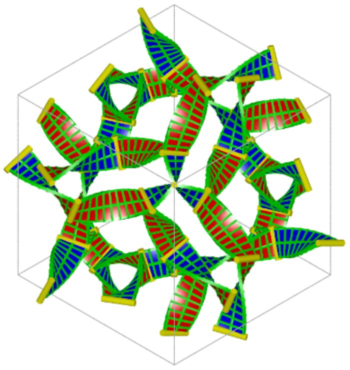
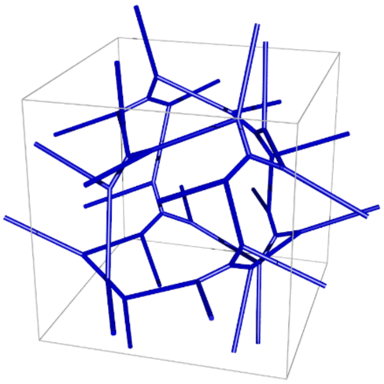
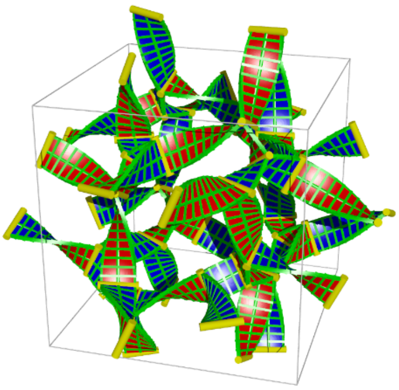
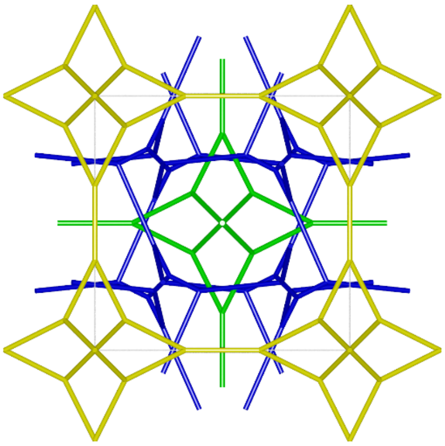
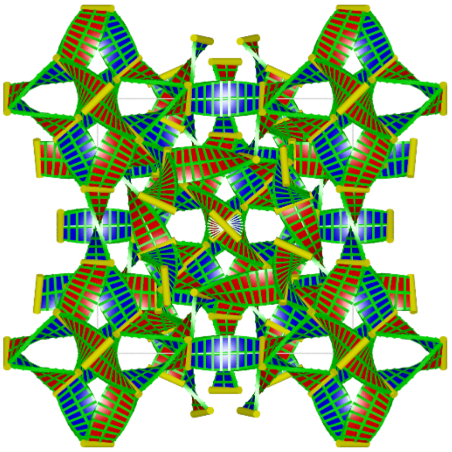
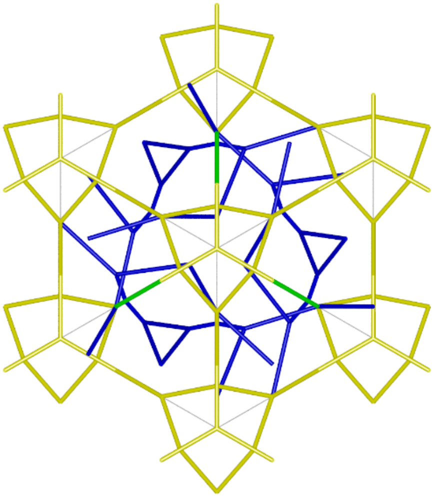
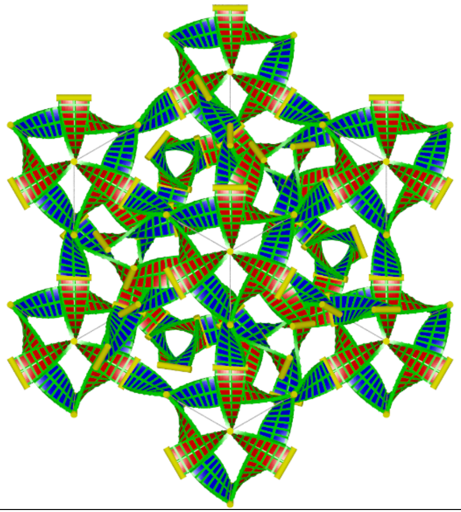
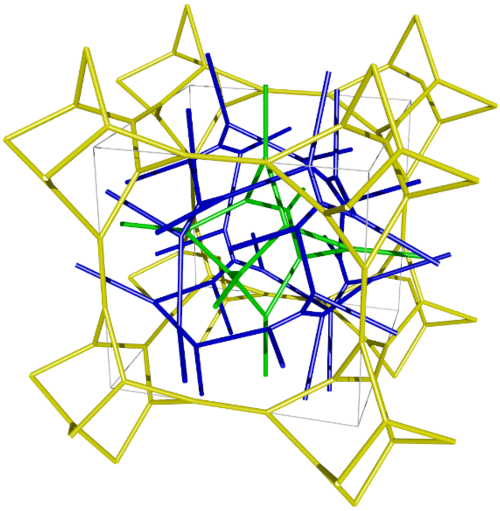
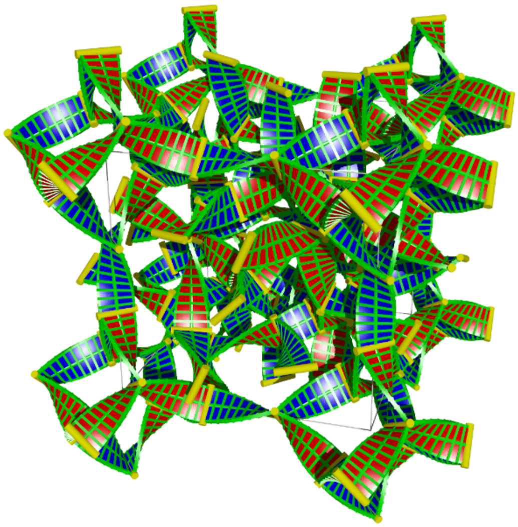
	Rods	Ribbons
View along (100)		
View along (111)		
Oblique view		

Figure S5. All networks different views

	Rods	Ribbons
View along (100)		
View along (111)		
Oblique view		

S3. Calculation of the structure factor $F(hkl)$

The structural factor *F*(*hkl*) is linked to the electron density ρ(*uvw*), where *u*,*v*,*w* are the fractional coordinates in the unit cell, by Fourier transform

$$F(hkl) = \int_0^1 \int_0^1 \int_0^1 \rho(uvw) \exp[\mathrm{i}2\pi(hu + kv + lw)] du dv dw \qquad (Equation\ S1)$$

$F(hkl)$ is a complex number and has a real part, $A(hkl)$ and an imaginary part, $B(hkl)$

$$F(hkl) = |F(hkl)| \exp[i\phi(hkl)] = A(hkl) + iB(hkl) \qquad (Equation\ S2)$$

Equation S1 can thus be rewritten as

$$A(hkl) = \int_0^1 \int_0^1 \int_0^1 \rho(uvw) \cos[2\pi(hu + kv + lw)] du dv dw \qquad (Equation\ S3a)$$

$$B(hkl) = \int_0^1 \int_0^1 \int_0^1 \rho(uvw) \sin[2\pi(hu + kv + lw)] du dv dw \qquad (Equation\ S3b)$$

Using the above equations, we have calculated the diffraction intensities and phases for each observed peak from the Fourier transform of the model, where the electron density of a point $\rho(uvw)$ in the unit cell is taken to be 1 when its distance to the nearest network segment is less than a constant value R, and 0 otherwise. The R constant defines the boundary between high and low electron density regions of the phase, and it is chosen to be 0.09*a* so that the high electron density regions occupy 45% of the total volume, where 45% is the volume ratio of the rigid aromatic core of the compound under study (compound 1**e**, ref. S3). The unit cell is divided in all three dimensions by 200 times, and the integration is approximated by summation

$$A(hkl) = \frac{C}{8000000} \sum_{u=0.005}^{1} \sum_{v=0.005}^{1} \sum_{w=0.005}^{1} \rho(uvw) \cos[2\pi(hu + kv + lw)] \qquad (Equation\ S4a)$$

$$B(hkl) = \frac{C}{8000000} \sum_{u=0.005}^{1} \sum_{v=0.005}^{1} \sum_{w=0.005}^{1} \rho(uvw) \sin[2\pi(hu + kv + lw)] \qquad (Equation\ S4b)$$

Here C=250 is a constant used so that the calculated values are more tractable. The calculated $A(hkl)$ and $B(hkl)$ values, relative intensities $I(hkl) = |F(hkl)|^2 = A(hkl)^2 + B(hkl)^2$, and phase angles $\phi(hkl)$ are shown in Table S1. In reconstruction of electron density map from experimental data, the phase angles, and the intensity ratios $I(hkl)/I(hlk)$ are taken to be the same as calculated.

Table S1. Calculated intensities and phase angles of diffraction peaks of the $I23$ phase.

(hkl)	$A(hkl)$	$B(hkl)$	$I(hkl)$	$\phi(hkl)$
(110)	2.92	0.00	8.5	0
(200)	-9.38	0.00	88.0	π
(211)	-4.96	-0.52	24.8	-0.97π
(220)	1.80	0.00	3.3	0
(310)	0.85	0.00	0.7	0
(301)	6.40	0.00	41.0	0
(222)	4.08	-3.79	31.1	-0.24π
(321)	-8.00	-2.23	69.0	-0.91π
(312)	-3.46	-11.85	152.3	-0.59π
(400)	11.59	0.00	134.3	0
(411)	-5.76	-3.86	48.1	-0.81π
(330)	7.27	0.00	52.9	0
(420)	6.19	0.00	38.4	0
(402)	0.71	0.00	0.5	π
(332)	-0.71	2.72	7.9	0.58π
(422)	-0.68	-1.24	2.0	-0.66π

References

S1. Zeng, X. B., Ungar, G. and Imperor-Clerc, *Nature Materials*, 2005, **4**, 562-567.

S2. Ozawa, K., Yamamura, Y., Yasuzuka, S., Mori, H., Kutsumizu, S. and Saito, *J. Phys. Chem B.*, 2008, **112**, 12179–12181.

S3. C. Dressel, F. Liu, M. Prehm, X. B. Zeng, G. Ungar and C. Tschierske, *Angew. Chem. Int. Ed.*, 2014, **126**, 13331-13336.