

SUPPORTING INFORMATION FOR
Close-Packed Dye Molecules in Zeolite Channels Self-assemble into Supramolecular
Nanoladders

Lara Gigli¹, Rossella Arletti^{2,3}, Gloria Tabacchi^{4*}, Ettore Fois⁴, Jenny G. Vitillo^{3,4}, Gianmario Martra^{3,5}, Giovanni Agostini^{3,5‡}, Simona Quartieri⁶, Giovanna Vezzalini¹

¹ Dipartimento di Scienze Chimiche e Geologiche, Università degli Studi di Modena e Reggio Emilia, Via Giuseppe Campi 183, 41125- Modena, Italy

² Dipartimento di Scienze della Terra, Università degli Studi di Torino, Via Valperga Caluso 35, 10125-Torino, Italy.

³ Interdepartmental Centre “Nanostructure Interfaces and Surfaces – NIS”, Via Pietro Giuria 7, 10125-Torino, Italy.

⁴ Dipartimento di Scienza ed Alta Tecnologia, Università degli Studi dell’Insubria, Via Lucini 3, 22100-Como, Italy

⁵ Dipartimento di Chimica, Università degli Studi di Torino, Via Pietro Giuria 7, 10125-Torino, Italy.

⁶ Dipartimento di Fisica e Scienze della Terra, Università degli Studi di Messina, Viale Ferdinando Stagno d’Alcontres 3, 98166-Messina S.Agata, Italy

[‡]Present address: European Synchrotron Radiation Facility (ESRF), B.P. 220, 38043 Grenoble, France

* corresponding author

Figure S1. Observed and calculated diffraction patterns and final difference curve from Rietveld refinements of the pure ZL and of the ZL/0.5FL, ZL/1.0FL, ZL/1.5FL composites.

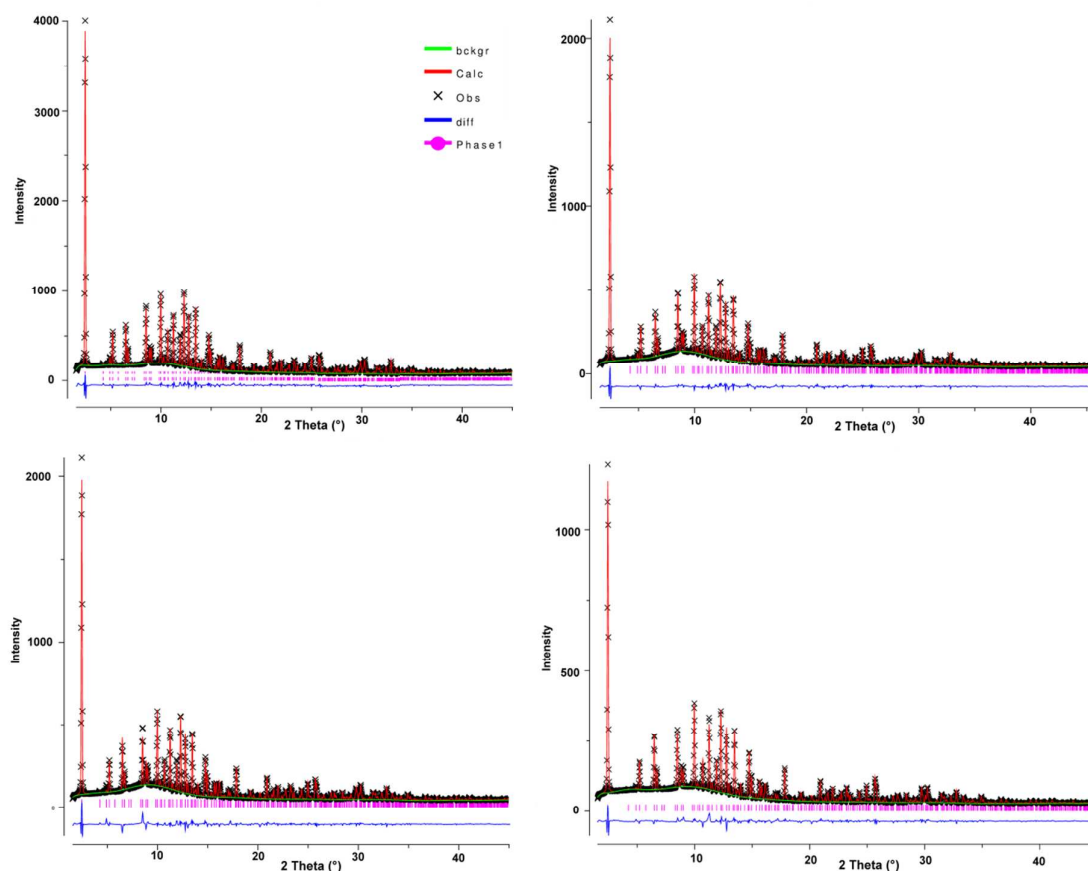


Figure S2. ATR-IR spectra, normalized to the peak at ca. 1005 cm^{-1} , of bare ZL (dot, black line) and ZL/FL materials having 0.5 (light gray), 1.0 (gray), and 1.5 FL molecules/u.c. (solid black) loadings before (section a) and after (section b) thermal treatment.

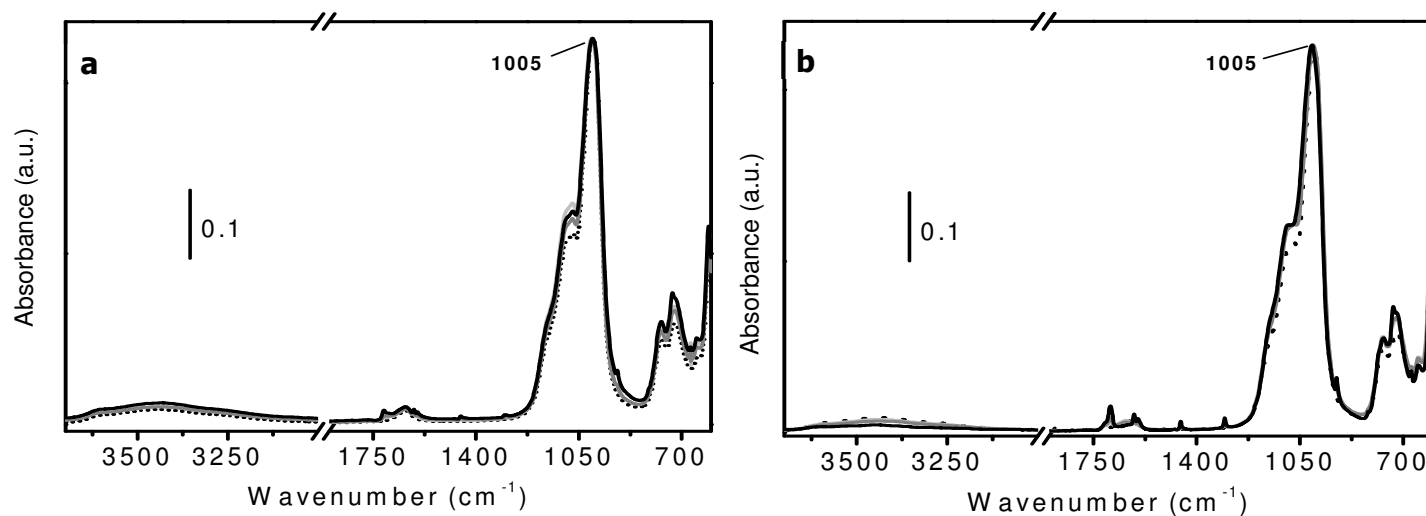


Table S1. Atomic coordinates, occupancy factors and thermal displacement parameters for the structures of the ZL, ZL/0.5FL, ZL/1.0FL and ZL/1.5FL composites.

Atom	x/a	y/b	z/c	Occ.	Uiso
ZL					
T1	0.0939(1)	0.3566(2)	0.5	1	0.0136(5)
T2	0.1646(2)	0.4978(1)	0.2093(2)	1	0.0136(5)
O1	0	0.2694(6)	0.5	1	0.0159(9)
O2	0.1616(2)	0.3233(5)	0.5	1	0.0159(9)
O3	0.2671(2)	0.5342(4)	0.2534(8)	1	0.0159(9)
O4	0.1019(3)	0.4127(3)	0.3241(5)	1	0.0159(9)
O5	0.4245(2)	0.8490(4)	0.2645(9)	1	0.0159(9)
O6	0.1452(4)	0.4762(4)	0	1	0.0159(9)
KB	0.33333	0.66667	0.5	1	0.016(3)
KC	0.5	0	0.5	1	0.37(3)
KD	0.3006(5)	0	0	0.804(2)	0.57(3)
WF	0.117(2)	0	0	0.42(1)	0.149(9)
WH	0.119(1)	0	0.371(2)	0.43(1)	0.149(9)
WI	0.257(1)	0.128(5)	0	0.88(1)	0.149(9)
WJ	0.162(1)	0.0814(7)	0.292(3)	0.44(1)	0.149(9)
WK	0	0	0.185(1)	0.25(2)	0.149(9)
ZL/0.5FL					
T1	0.0933(3)	0.3583(3)	0.5	1	0.015(6)
T2	0.1660(2)	0.4994(2)	0.2107(4)	1	0.015(6)
O1	0	0.2746(8)	0.5	1	0.017(1)
O2	0.1653(4)	0.3308(9)	0.5	1	0.017(1)
O3	0.2641(3)	0.5284(7)	0.250(1)	1	0.017(1)
O4	0.1038(4)	0.4151(4)	0.3242(8)	1	0.017(1)
O5	0.4282(1)	0.8564(4)	0.266(1)	1	0.017(1)
O6	0.1457(7)	0.4777(6)	0	1	0.017(1)
KB	0.33333	0.66667	0.5	1	0.022(4)
KC	0.5	0	0.5	1	0.045(4)
KD	0.3020(6)	0	0	0.820(8)	0.067(4)
WH	0.158(3)	0	0.196(5)	0.313(7)	0.115(3)
FL					
C1	0.0251(4)	0.0125(2)	0.4060(7)	0.080(1)	0.175(5)
C2	0.1069(3)	0.0535(2)	0.4615(7)	0.080(1)	0.175(5)
C3/WJ	0.1694(3)	0.0847(1)	0.3337(1)	0.60(4)	0.175(5)
C4	0.1434(5)	0.0717(2)	0.1559(3)	0.080(1)	0.175(5)
C5	0.0594(4)	0.0297(2)	0.0957(2)	0.080(1)	0.175(5)
C6	0	0	0.3337(1)	0.50(3)	0.175(5)
C7	0.1978(4)	0.0989(2)	0	0.080(1)	0.175(5)
OFL/WI	0.2728(5)	0.1364(2)	0	0.89(1)	0.175(5)
ZL/1.0FL					
T1	0.0934(3)	0.3575(3)	0.5	1	0.012(5)
T2	0.1658(3)	0.4989(2)	0.2108(4)	1	0.012(5)
O1	0	0.2746(8)	0.5	1	0.016(1)
O2	0.1640(5)	0.3280(9)	0.5	1	0.016(1)
O3	0.2645(3)	0.5289(7)	0.248(2)	1	0.016(1)

O4	0.1022(5)	0.4168(4)	0.3298(8)	1	0.016(1)
O5	0.4263(2)	0.8525(4)	0.268(2)	1	0.016(1)
O6	0.1462(7)	0.4801(7)	0	1	0.016(1)
KB	0.33333	0.66667	0.5	1	0.016(2)
KC	0.5	0	0.5	1	0.034(2)
KD	0.3071(7)	0	0	0.871(9)	0.073(2)
<i>FL</i>					
C1	0.0287(3)	0.0143(2)	0.4079(6)	0.158(1)	0.197(5)
C2	0.1105(3)	0.0553(2)	0.4635(6)	0.158(1)	0.197(5)
C3/WJ	0.1707(2)	0.0854(1)	0.3306(1)	0.631(1)	0.197(5)
C4	0.1415(4)	0.0708(2)	0.1556(2)	0.158(1)	0.197(5)
C5	0.0575(4)	0.0287(2)	0.0957(2)	0.158(1)	0.197(5)
C6	0	0	0.2333(6)	1.00(4)	0.197(5)
C7	0.1961(4)	0.0980(2)	0	0.158(1)	0.197(5)
OFL/WI	0.2712(4)	0.1356(2)	0	0.81(2)	0.197(5)
ZL/1.5FL					
T1	0.0943(4)	0.3587(3)	0.5	1	0.016(5)
T2	0.1667(3)	0.5004(3)	0.2100(4)	1	0.016(5)
O1	0	0.2770(8)	0.5	1	0.018(1)
O2	0.1640(5)	0.3281(9)	0.5	1	0.018(1)
O3	0.2650(4)	0.5299(7)	0.253(2)	1	0.018(1)
O4	0.1031(5)	0.4185(4)	0.3303(9)	1	0.018(1)
O5	0.4283(2)	0.8567(4)	0.269(2)	1	0.018(1)
O6	0.1457(8)	0.4791(7)	0	1	0.018(1)
KB	0.33333	0.66667	0.5	1	0.016(3)
KC	0.5	0	0.5	1	0.032(3)
KD	0.3127(6)	0	0	0.845(9)	0.085(3)
<i>FL</i>					
C1	0.0312(3)	0.0156(8)	0.4095(5)	0.080(1)	0.17(4)
C2	0.1134(4)	0.0567(2)	0.4634(5)	0.080(1)	0.17(4)
C3/WJ	0.1718(6)	0.0859(3)	0.3268(4)	0.43(4)	0.17(4)
C4	0.1409(4)	0.0704(6)	0.1550(2)	0.080(1)	0.17(4)
C5	0.0570(6)	0.0285(3)	0.0960(6)	0.080(1)	0.17(4)
C6	0	0	0.2362(2)	0.50(3)	0.17(4)
C7	0.1959(4)	0.0979(5)	0	0.08(1)	0.17(4)
OFL/WI	0.2709(3)	0.1355(4)	0	0.58 (1)	0.17(4)
<i>FL'</i>					
C'1	0.0999(6)	0.0499(5)	0.3306(4)	0.164(1)	0.17(4)
C'2	0.1261(9)	0.1261(9)	0.4237(7)	0.164(1)	0.17(4)
C'3	0.2033(2)	0.0513(5)	0.3430(4)	0.082(1)	0.17(4)
C'4	0.2085(5)	0.1460(5)	0.1615(6)	0.082(1)	0.17(4)
C'5	0.1322(3)	0	0.0928(2)	0.164(1)	0.17(4)
C'6	0.1130(5)	0.0565(6)	0.1471(3)	0.164(1)	0.17(4)
C'7	0.258(1)	0.0978(3)	0	0.082(1)	0.17(4)
O'FL	0.325(1)	0.1625(4)	0	0.164(1)	0.17(4)

Table S2. Framework bond distances for the ZL and ZL/0.5FL, ZL/1.0FL and ZL/1.5FL composites

	ZL	ZL/0.5FL	ZL/1.0FL	ZL/1.5FL
T1-O1	1.635(4)	1.632(4)	1.630(3)	1.633(4)
O2	1.632(4)	1.637(3)	1.638(3)	1.642(4)
O4 [X2]	1.635(3)	1.634(3)	1.636(2)	1.639(3)
average	1.634	1.634	1.635	1.638
T2-O3	1.643(4)	1.633(3)	1.636(3)	1.640(4)
O4	1.642(4)	1.636(3)	1.640(3)	1.643(4)
O5	1.624(4)	1.631(5)	1.630(6)	1.634(6)
O6	1.624(3)	1.632(3)	1.624(3)	1.625(3)
average	1.633	1.633	1.633	1.64

Table S3. Extraframework bond distances < 3.2 Å for the ZL, ZL/0.5FL, ZL/1.0FL and ZL/1.5FL composites.

ZL			ZL/0.5FL			ZL/1.0FL			ZL/1.5FL		
KB-	O3 [x6]	2.884(9)	KB-	O3 [x6]	2.89(1)	KB-	O3 [x6]	2.90(1)	KB-	O3 [x6]	2.86(1)
KC-	O5 [x4]	2.985(8)	KC-	O5 [x4]	2.89(1)	KC-	O5 [x4]	2.93(1)	KC-	O5 [x4]	2.87(1)
KD-	O4 [x4]	3.146(6)	KD-	O4 [x4]	3.158(4)	KD-	O4 [x4]	3.166(4)	KD-	O4 [x4]	3.140(4)
	O6 [x2]	3.033(5)		O6 [x2]	3.012(6)		O6 [x2]	2.983(7)		O6 [x2]	2.893(7)
	WI [x2]	2.848(6)		OFL/WI[x2]	2.809(6)		OFL/WI[x2]	2.864(7)		O'FL[x2]	2.887(5)
WF-	WF [x2]	2.13(3)		WH [x2]	3.008(8)	OFL/WI	C3[x2]	2.96(2)		OFL/WI[x2]	2.957(8)
	WH [x2]	2.81(2)	WH-	O1	2.832(4)		C7	1.20(2)		C7'[x2]	2.466(9)
	WI [x2]	2.47(2)		C2 [x2]	2.64(4)	WJ/C3-	O2	2.84(1)		C4'[x2]	2.948(9)
	WJ [x4]	2.56(2)		C2 [x2]	3.11(4)		C4	1.39(3)	OFL/WI-	C6'[x2]	2.56(3)
	WK [x2]	2.60(3)		C5 [x2]	2.29(4)		C4[x2]	2.84(3)		C4'[x4]	1.64(1)
WH-	O1	2.98(1)		C5 [x2]	3.18(4)		C2[x2]	2.59(3)		C4[x2]	2.20(3)
	WF	2.81(2)		C5 [x2]	3.07(4)		C2[x2]	3.03(2)		C5'[x4]	2.45(3)
	WH[x2]	2.20(2)		C4 [x2]	3.01(4)		C2[x2]	3.20(2)		OFL'	1.07(4)
	WH[x2]	2.91(3)		C4 [x2]	1.53(3)		C2	2.34(3)		C3'[x4]	2.87(1)
	WH	1.91(4)		WH [x2]	2.94(4)		C2	3.00(3)		C7'[x2]	0.78(7)
	WJ[x2]	1.425(8)		WH	2.89(8)		C5[x2]	2.98(4)		C3/WJ[x2]	2.81(1)
	WJ[x2]	2.83(2)		OFL[x2]	2.74(3)		C5	2.52(3)		C7	1.21(4)
	WK	2.60(2)		C3/WJ[x2]	1.83(3)		OFL/WI	2.95(3)		C'7	0.60(4)
WI-	WF[x2]	2.47(2)		C1[x2]	3.07(4)		C3/WJ[x2]	2.71(3)	C3/WJ-	O2	3.12(6)
	WJ[x2]	2.675(9)		C7[x2]	2.15(3)		C3/WJ	2.55(3)		C3'[x2]	1.31(4)
WJ-	O2	3.06(1)	OFL/WI	C4 [x2]	2.37(1)		C5	2.52(3)		C3'[x2]	2.52(2)
	WF[x2]	2.56(2)		C5[x2]	3.15(2)		C5[x2]	2.97(3)		C3'[x2]	2.82(4)
	WH[x2]	1.425(8)		WH[x4]	2.73(1)		C1[x2]	2.59(4)		C1[x2]	2.95(5)
	WH[x2]	2.83(2)		C3[x2]	3.00(1)		C1[x2]	2.84(3)		C1	2.47(6)
	WI	2.675(9)		C7	1.19(2)		C1	1.39(3)		C2'	2.02(5)
	WJ [x2]	2.59(2)	WJ/C3-	O2	2.85(2)		C1	1.82(3)		C2' [x2]	2.95(5)
	WJ	3.12(5)		C4	1.39(2)		C7	2.52(2)		C'2	2.83(5)
	WK	2.69(2)		C4[x2]	2.85(2)		C6	2.82(3)		C2[x2]	3.04(5)
WK-	WF [x6]	2.60(3)		C2[x2]	2.58(2)					C2	2.02(6)
	WH [x6]	2.60(2)		C2[x2]	2.96(2)					C2	2.50(6)
	WJ [x6]	2.69(2)		C2[x2]	3.19(2)					C1'[x2]	2.58(4)
	WK	2.85(2)		C2	2.37(2)					C1'[x2]	1.45(5)
				C2	3.02(2)					C4'[x2]	2.60(1)
				C5[x2]	2.96(2)					C4'[x2]	1.65(6)
				C5	2.50(2)					C4[x2]	2.66(3)
				OFL/WI	3.17(2)					C4	1.39(6)
				C3/WJ[x2]	2.70(1)					C5'[x2]	2.83(6)
				C3/WJ	2.50(2)					C5[x2]	2.72(5)
				C5	2.50(2)					C5	2.19(5)
				C5[x2]	2.96(2)					C5	3.14(6)
				C1[x2]	2.55(2)					C5	2.84(5)
				C1[x2]	2.82(2)					C6'[x2]	2.57(4)
				C1	1.38(2)					C6'	1.68(5)
				C1	1.83(2)					C7'[x2]	2.24(5)
				C7	2.55(2)					O'FL	2.89(5)
				WH	1.82(2)						
				C6	2.81(2)						