Supporting Information

Crosslinking rapidly cured epoxy resin thermosets: experimental and computational modeling and simulation study

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Table S1. Atom charges of molecules used in the computational modeling based on RED Methodology.

	TFSI			MDA				DGEBA				
S/N	Atom	Charge	S/N	Atom	Charge	S/N	Atom	Charge	S/N	Atom	Charge
1	C1	0.4438	1	C1	-0.1871	1	O1	-0.3533	30	H30	0.1002
2	S2	0.7571	2	H2	0.1892	2	O2	-0.3502	31	H31	0.1002
3	F3	-0.1292	3	C3	-0.2885	3	O3	-0.3949	32	C32	-0.1314
4	F4	-0.1370	4	H4	0.1712	4	O4	-0.3757	33	H33	0.1547
5	F5	-0.1489	5	C5	0.3879	5	C5	0.1616	34	C34	-0.1614
6	N6	-0.7125	6	C6	-0.2988	6	C6	-0.0068	35	H35	0.1585
7	O7	-0.4851	7	H7	0.1818	7	H7	0.1440	36	C36	-0.1602
8	O8	-0.4954	8	C8	-0.1933	8	C8	-0.0237	37	H37	0.1658
9	S9	0.9449	9	H9	0.1544	9	H9	0.1496	38	C38	-0.1638
10	C10	0.2922	10	C10	0.0283	10	C10	-0.0394	39	H39	0.1626
11	O11	-0.5247	11	C11	-0.2598	11	C11	-0.0215	40	C40	0.3364
12	O12	-0.5101	12	H12	0.1729	12	C12	-0.0827	41	C41	0.2898
13	F13	-0.0932	13	C13	-0.2202	13	H13	0.1285	42	C42	-0.2535
14	F14	-0.1339	14	H14	0.1613	14	H14	0.1285	43	H43	0.1527
15	F15	-0.0680	15	C15	0.0378	15	C15	-0.072	44	C44	-0.2123
			16	C16	-0.1988	16	H16	0.1261	45	H45	0.1445
			17	H17	0.1908	17	H17	0.1261	46	C46	-0.2478
			18	C18	-0.2633	18	C18	-0.1556	47	H47	0.1107
			19	H19	0.1677	19	H19	0.0422	48	C48	-0.2266
			20	C20	0.3462	20	H20	0.0422	49	H49	0.1086
			21	C21	-0.0255	21	H21	0.0422			
			22	H22	0.0407	22	C22	-0.156			
			23	H23	0.0407	23	H23	0.0419			
			24	N24	-0.8843	24	H24	0.0419			
			25	H25	0.3604	25	H25	0.0419			
			26	H26	0.3604	26	C26	0.1102			
			27	N27	-0.8859	27	H27	0.0932			
			28	H28	0.3569	28	H28	0.0932			
			29	H29	0.3569	29	C29	0.0908			

Table S2. Atom charges of Li@3G with DGEBA used in the computational modeling based on MCPB Methodology.

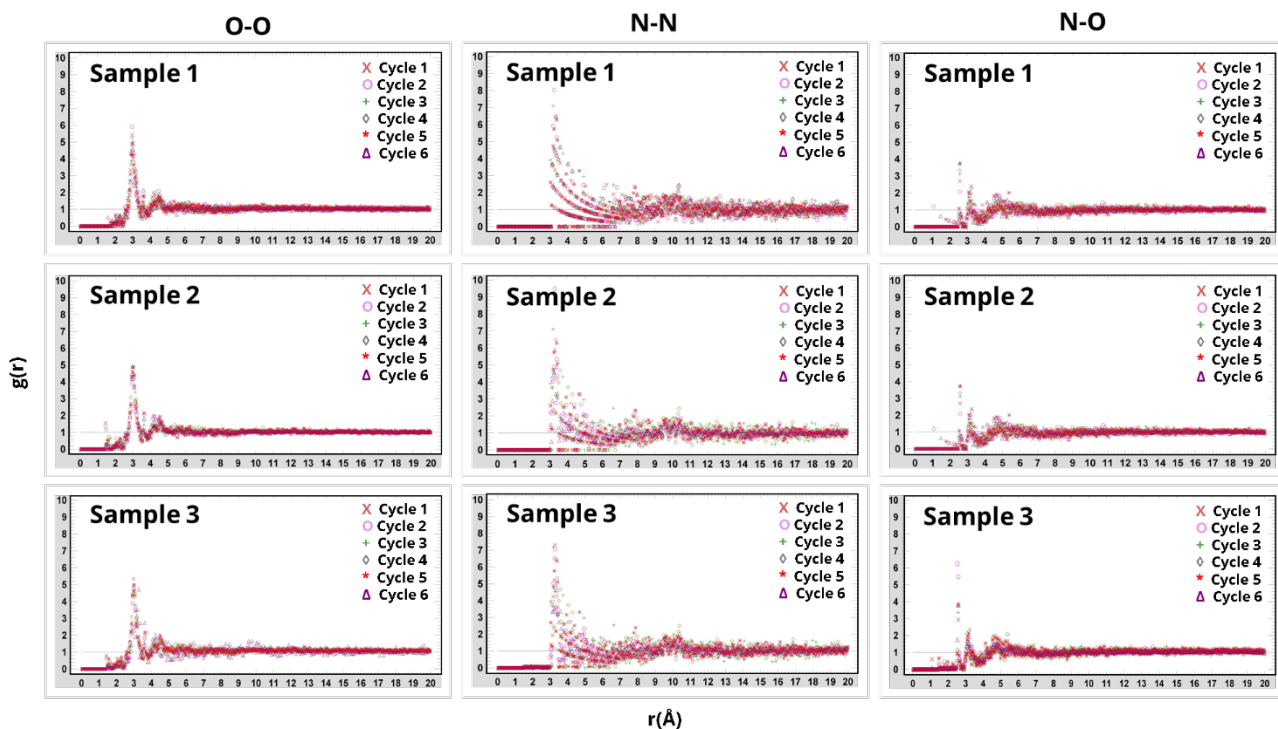| S/N	Atom	Charge	S/N	Atom	Charge	S/N	Atom	Charge	S/N	Atom	Charge
					Li@G3 with DGEBA						
1	**C1**	-0.0982	21	**H21**	0.0567	41	**C41**	0.3744	61	**O61**	-0.4076
2	**H2**	0.0835	22	**H22**	0.0567	42	**C42**	-0.362	62	**C62**	0.2658
3	**H3**	0.0835	23	**C23**	0.0202	43	**H43**	0.0855	63	**H63**	0.0017
4	**H4**	0.0835	24	**H24**	0.0633	44	**H44**	0.0855	64	**H64**	0.0017
5	**O5**	-0.1628	25	**H25**	0.0633	45	**H45**	0.0855	65	**C65**	0.0855
6	**C6**	-0.0621	26	**O26**	-0.2566	46	**C46**	-0.3668	66	**H66**	0.0231
7	**H7**	0.0756	27	**C27**	-0.1253	47	**H47**	0.0868	67	**H67**	0.0231
8	**H8**	0.0756	28	**H28**	0.0883	48	**H48**	0.0868	68	**C68**	0.4944
9	**C9**	0.0276	29	**H29**	0.0883	49	**H49**	0.0868	69	**H69**	-0.036
10	**H10**	0.0672	30	**H30**	0.0883	50	**C50**	-0.2351	70	**C70**	0.5474
11	**H11**	0.0672	31	**C31**	-0.0918	51	**H51**	0.1505	71	**H71**	-0.0795
12	**O12**	-0.1681	32	**H32**	0.118	52	**C52**	-0.1666	72	**O72**	-0.4436
13	**C13**	-0.0966	33	**C33**	-0.3029	53	**H53**	0.1185	73	**O73**	-0.846
14	**H14**	0.0814	34	**H34**	0.1494	54	**C54**	0.006	74	**C74**	-0.4199
15	**H15**	0.0814	35	**C35**	0.3819	55	**C55**	-0.181	75	**H75**	0.1096
16	**C16**	0.1147	36	**C36**	-0.2562	56	**H56**	0.1227	76	**H76**	0.1096
17	**H17**	0.0616	37	**H37**	0.1187	57	**C57**	-0.2255	77	**C77**	-0.1992
18	**H18**	0.0616	38	**C38**	-0.1242	58	**H58**	0.1396	78	**H78**	0.0703
19	**O19**	-0.3474	39	**H39**	0.1282	59	**C59**	0.3548	79	**H79**	0.0703
20	**C20**	0.0542	40	**C40**	-0.0636	60	**O60**	-0.3797	80	**Li1**	0.4783

Figure S1. Evaluation of the RDFs calculated for the liquid mixture as a function of the six simulated annealing cycles.

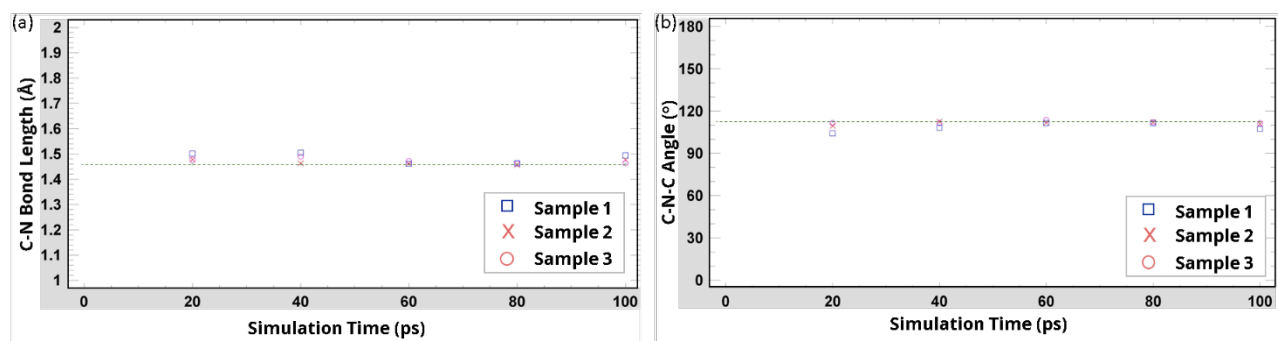**Figure S2.** (**a**) Bond lengths of the crosslink bonds, and (**b**) bond angles between the C-N-C atoms of the crosslink bonds for equilibrated crosslinked samples at 81.0 % crosslinking degree. The dashed lines represent the AMBER Force Field ideal values.
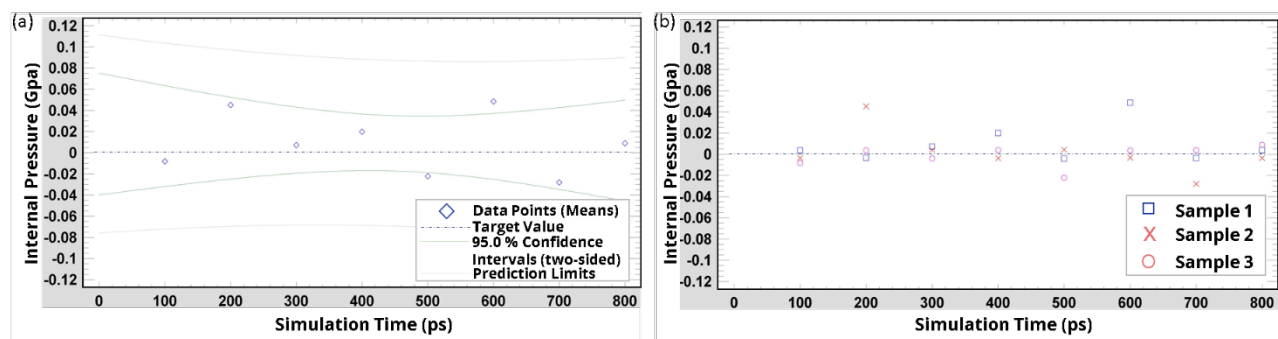

Figure S3. (**a**) Calculated average internal pressure of the sample after the crosslinking process, and (**b**) the internal pressure of the three crosslinked samples. The dashed line represents the target pressure, 0.0001 GPa.