Supporting Information

A Computational Procedure for Atomistic Modelling of Polyphosphazenes towards Better Capturing Molecular-level Structuring and Thermo-mechanical Properties

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Partial atomic charges

Figure S1. Partial atomic charges used for (a) PZ-DC, (b) PZ-TFE, (c) PZ-Nitrato, (d) PZ-Azido.

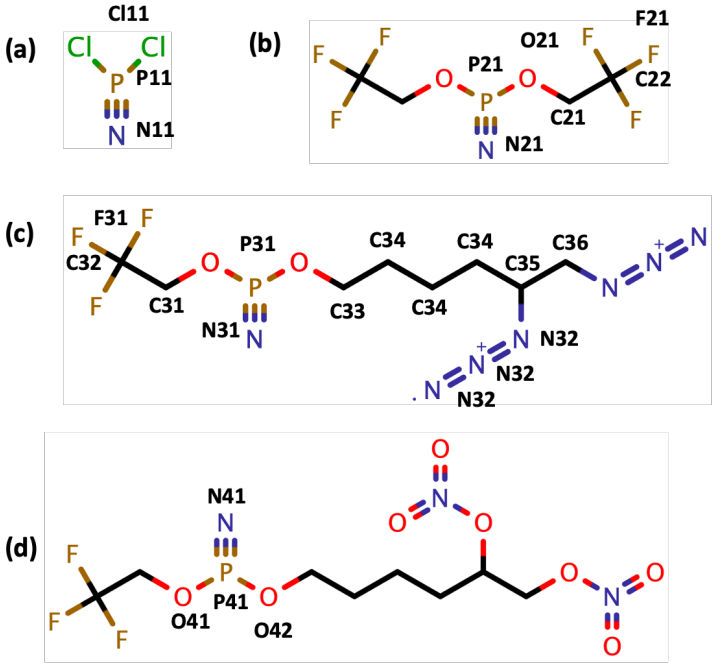


Table S1. List of the partial atomic charges for the unique atomic sites for the PZ-DC (the labels corresponding to Figure S1).

Label	q / esu
P11	0.1044
N11	0.0706
Cl11	-0.0875

Table S2. List of the partial atomic charges for the unique atomic sites for the PZ-TFE (the labels corresponding to Figure S1).

Label	q / esu	Label	q / usu
P21	0.0390	**C22**	0.1841
N21	0.0788	**F21**	-0.0981
O21	-0.2526	**H21**	0.1708
C21	-0.0377		

Table S3. List of the partial atomic charges for the unique atomic sites for the PZ-Azido (the labels corresponding to Figure S1).

Label	q / esu	Label	q / usu
P31	0.0493	**C36**	-0.1503
N31	0.0432	**N32**	-0.0550
O31	-0.2952	**F31**	-0.1176
O32	-0.3181	**H31**	0.1535
C31	-0.0270	**H33**	0.1487
C32	0.1478	**H34**	0.1416
C33	-0.0063	**H35**	0.1441
C34	-0.2158	**H36**	0.1455
C35	-0.0023		

Table S4. List of the partial atomic charges for the unique atomic sites for the PZ-Nitrato (the labels corresponding to Figure S1).

Label	q / esu	Label	q / usu
P41	0.0432	**N42**	0.8215
N41	0.0837	**O43**	-0.5148
O41	-0.2570	**O44**	-0.4042
O42	-0.3022	**F41**	-0.0994
C41	-0.0354	**H41**	0.1689
C42	0.1832	**H43**	0.1453
C43	-0.0186	**H44**	0.1582
C44	-0.2213	**H45**	0.1821
C45	0.1514	**H46**	0.1706
C46	0.0163		

Table S5. Bond length and bond force constants used for relaxing newly formed bonds between the monomers for each system.

Step	r_0 / Å	k_b / kcal.mol^{-1}	Step	r_0 / Å	k_b / kcal.mol^{-1}
1	6.00	1	**11**	3.50	140
2	5.75	2	**12**	3.25	160
3	5.50	5	**13**	3.00	180
4	5.25	10	**14**	2.75	200
5	5.00	20	**15**	2.50	225
6	4.75	40	**16**	2.25	250
7	4.50	60	**17**	2.00	275
8	4.25	80	**18**	1.75	300
9	4.00	100	**19**	1.495	325
10	3.75	120	**20**	1.495	350

Figure S2. (a) Tensile stress-strain curves (SSCs) for the polymerised systems obtained at 20 ^{o}C. (b) A zoomed-in version of (a). The lines represent the fit lines used to calculate the Young's modulus, up to a strain of 2 %.

