

Positive effect of functional side groups on the structure and properties of benzoxazine networks and nanocomposites

Shamil Saiev^a, Leïla Bonnaud^b, Camilo Zúñiga^{b,c}, Philippe Dubois^b, David Beljonne^a, J.C. Ronda^c, V. Cadiz^c, Roberto Lazzaroni^{a*}

^a *Laboratory for Chemistry of Novel Materials, Materials Research Institute, University of Mons – UMONS, Place du Parc 20, 7000 Mons (Belgium)*

^b *Laboratory of Polymeric and Composite Materials, Center of Innovation and Research in Materials and Polymers (CIRMAP), Materia Nova Research Center & University of Mons, Place du Parc 20, 7000 Mons (Belgium)*

^c *Departament de Química Analítica i Química Orgànica, Universitat Rovira i Virgili, Campus Sescelades, Marcel·lí Domingo s/n, 43007 Tarragona (Spain)*

Supplementary Information

The modified parameters of the Dreiding forcefield are regrouped in Tables S1 and S2.

Table S1. Modified dihedral parameters for Dreiding forcefield.

C_R	C_R	C_3	X	Dihedral	20	-1	3
C_R	O_R	C_3	H_	Dihedral	1	1	2
C_R	O_R	C_3	X	Dihedral	5	1	2
H_	C_3	N_3	C_R	Dihedral	12.5	1	2
X	N_3	C_3	X	Dihedral	5	-1	5
X	N_3	C_R	C_R	Dihedral	11	1	2
X	N_3	C_R	X	Dihedral	5	1	2
X	O_R	C_R	X	Dihedral	8	1	3
X	O_R	C_3	X	Dihedral	7	1	2

Table S2. Modified van der Waals parameters for Dreiding forcefield.

F _i	F _j	Functional Form	D0/kcal/mol	R0/Å
H_	H_	L_J_12_6	0.0152	2.8

For details on the optimization procedure of the force field, refer to the supplementary information provided in our previous work [S1], which also provides the justification for the size of the CNTs used in the simulations.

- 1 S1. Saiev, S.; Bonnaud, L.; Dumas, L.; Zhang, T.; Dubois, P.; Beljonne, D.; Lazzaroni, R. Do Carbon Nanotubes Improve the Thermomechanical Properties of Benzoxazine Thermosets? *ACS applied materials & interfaces* **2018**, *10* (31), 26669-26677.