

Supplementary Materials

A new framework for predicting tensile stress of natural rubber based on data augmentation and molecular dynamics simulation data

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The dataset comprises a total of 86 groups of tensile stress data for natural rubber. The feature values include the percentage of phospholipid protein (ω), hydrogen bonding strength (ϵ_H), and non-hydrogen bonding strength (ϵ_{NH}), with tensile stress serving as the target value. Specifically, the percentage of phospholipid protein ranges from 0.18% to 5.16%, with units in percentage (%); the hydrogen bonding strength ranges from 1.9 to 11.3 kcal/mol; and the non-hydrogen bonding strength ranges from 0.019 to 1.14 kcal/mol. The tensile stress ranges from 1200 to 3800 Pa. This experimental data was provided by the Advanced Elastomer Center at Beijing University of Chemical Technology.

Supplementary Table 1. Tensile stress data for natural rubber at 600% strain

Sample	ϵ_{NH}	ϵ_H	ω	Fn
1	0.38	1.9	0.18	1200.336
2	0.38	3.8	0.18	1298.7415
3	0.38	1.9	3.5	1322.8065
4	0.38	2	3.5	1328.3495
5	0.38	2.2	3.5	1414.4645
6	0.38	5.7	0.18	1484.2985
7	0.38	2.8	3.5	1571.8365
8	0.38	3.8	0.9	1583.312
9	0.38	2.85	3.5	1611.0365
10	0.38	7.6	0.18	1646.368
11	0.38	3.8	1.78	1656.303
12	0.95	9.5	0.18	1695.988
13	0.38	3.2	3.5	1704.684
14	0.38	3	3.5	1736.1145
15	0.38	9.5	0.18	1749.955
16	0.38	3.8	2.65	1776.208

17	0.38	3.8	3.5	1951.457
18	0.38	3.8	4.34	1986.1995
19	0.38	4.75	3.5	2095.5105
20	0.38	4	3.5	2096.7805
21	0.38	4.8	3.5	2186.8215
22	0.38	3.8	5.16	2191.299
23	0.38	5.2	3.5	2235.536
24	0.95	2.85	5.16	2302.0725
25	0.95	9.5	0.9	2322.891
26	0.95	1.9	5.16	2337.693
27	0.38	5.8	3.5	2382.9025
28	0.95	9.5	1.78	2410.4315
29	0.38	5.7	3.5	2454.315
30	0.076	7.6	3.5	2480.2475
31	0.38	6.65	3.5	2511.538
32	0.19	7.6	3.5	2558.937
33	0.57	7.6	3.5	2586.005
34	0.057	7.6	3.5	2597.798
35	0.38	5	3.5	2646.623
36	0.019	7.6	3.5	2655.459
37	0.152	7.6	3.5	2677.3485
38	0.95	3.8	5.16	2691.3765
39	0.38	7.6	3.5	2704.068
40	0.114	7.6	3.5	2718.3735
41	0.038	7.6	3.5	2722.259
42	0.133	7.6	3.5	2739.0635
43	0.95	9.5	2.65	2740.21
44	0.76	7.6	3.5	2740.8175
45	0.095	7.6	3.5	2862.264

46	0.95	6.65	5.16	2920.1995
47	0.38	8.55	3.5	2934.7415
48	0.38	9.5	5.16	2937.3315
49	0.95	9.5	3.5	2953.265
50	0.95	4.75	5.16	2958.491
51	0.665	9.5	5.16	2979.656
52	0.38	9.5	3.5	2990.915
53	0.38	10.4	3.5	2999.104
54	0.95	7.6	3.5	3102.077
55	0.19	9.5	5.16	3127.077
56	0.76	9.5	5.16	3230.2495
57	0.38	11.3	3.5	3231.382
58	0.95	5.7	5.16	3323.9385
59	0.95	7.6	5.16	3427.145
60	1.14	7.6	3.5	3429.2855
61	0.95	9.5	4.34	3467.304
62	0.855	9.5	5.16	3547.783
63	0.95	9.5	5.16	3625.017
64	0.95	8.55	5.16	3760.7145
65	0.38	7	4.8	2639.9181
66	0.38	7.3	4.8	2712.6872
67	0.38	7.6	4.8	2614.3792
68	0.38	7.9	4.8	2742.005
69	0.38	8.2	4.8	2710.1068
70	0.38	8.5	4.8	2784.0464
71	0.38	8.8	4.8	2888.2595
72	0.38	9.1	4.8	2787.166
73	0.38	5	5.7	2230.7073
74	0.38	5.3	5.7	2384.5475

75	0.38	5.6	5.7	2338.1447
76	0.38	5.9	5.7	2312.0948
77	0.38	6.2	5.7	2505.0071
78	0.38	6.5	5.7	2466.6935
79	0.38	6.8	5.7	2675.8793
80	0.38	7.1	5.7	2792.8668
81	0.38	2	1.78	1211.8315
82	0.38	2	2.65	1239.3165
83	0.38	2.5	1.78	1287.9035
84	0.38	2.5	2.65	1372.5411
85	0.38	3	1.78	1350.5927
86	0.38	3	2.65	1487.9448
