Supplementary Information

Study on the Brill transition of polyamide 6 with different crystal forms using low- and high-frequency Raman spectroscopy

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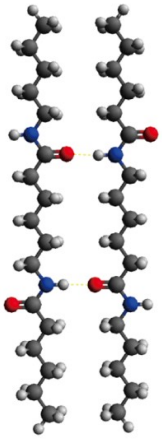
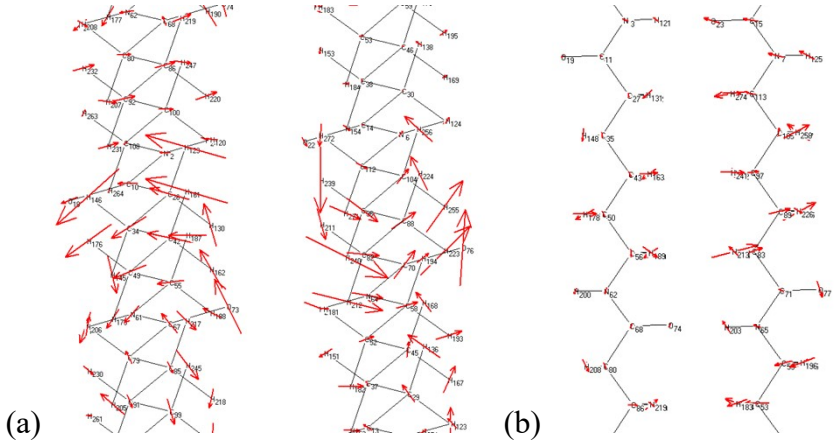


Fig. S1. A molecular fragment comprising two neighboring PA6 chains, each capped with methyl groups and consisting of two monomer units, used for optimization calculations. The resulting atomic tensors are subsequently transferred back to the original long chains.



(a) (b)

Fig. S2. Atomic motions of the Raman active modes of α-PA6 calculated at around (a) 70 cm^{-1} (overhead view along the c axis) and (b) 110 cm^{-1}.

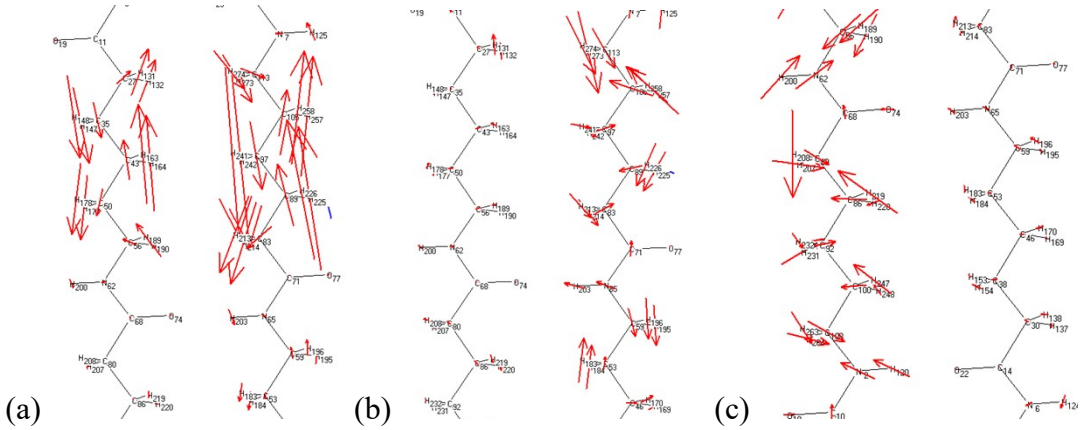


Fig. S3. Atomic motions of the Raman active modes of α-PA6 calculated at around (a) 1090 cm^{-1}, (b) 1105 cm^{-1} and (c) 1160 cm^{-1}.

Table S1. Optimized geometries of the PA6 fragment in Fig. S1.

No.	Atom	Geometry		
1	N	0.168002	4.971394	-0.212148
2	N	4.845998	3.661089	0.168546
3	C	-0.471478	3.828747	0.131258
4	C	4.251911	4.836821	-0.137011
5	O	-1.681104	3.77934	0.343797
6	O	3.122646	4.885275	-0.623245
7	C	0.421	2.607529	0.269271
8	C	5.086163	6.075087	0.136939
9	C	-0.296534	1.30741	-0.073436
10	C	4.317597	7.381483	-0.005486
11	C	0.591527	0.081435	0.120457
12	C	0.155411	17.47456	0.044434
13	C	5.188843	8.592565	0.315344
14	C	-0.500112	16.101025	-0.058711
15	C	4.468011	9.922324	0.118213
16	C	0.517486	14.973874	0.037376
17	C	5.348109	11.109215	0.486019
18	N	-0.135631	13.679958	-0.087087
19	N	4.661444	12.365457	0.261547
20	C	0.517269	12.511309	0.101247
21	C	5.332986	13.498532	-0.04762
22	O	1.706108	12.482473	0.416411
23	O	6.557666	13.540895	-0.144353
24	C	-0.316743	11.258653	-0.095934
25	C	4.463456	14.717943	-0.303449
26	C	0.464218	9.963176	0.077051
27	C	5.135701	16.020012	0.118974
28	C	-0.399911	8.738792	-0.210129
29	C	4.588081	-0.12933	-0.170294
30	C	4.289875	17.243643	-0.219906
31	C	0.339079	7.417318	-0.026126
32	C	5.229715	1.244517	0.008501
33	C	-0.542091	6.224427	-0.371184
34	C	4.208557	2.370884	-0.042179
35	C	-0.129981	-1.229542	-0.178111
36	C	5.603076	-1.266407	-0.112258
37	H	1.162247	4.941856	-0.416149
38	H	5.758189	3.679595	0.599319
39	H	0.762255	2.57534	1.31269
40	H	1.31528	2.7374	-0.346955
41	H	5.937132	6.0644	-0.55601
42	H	5.513382	5.995478	1.144348
43	H	-0.643685	1.347374	-1.113029
44	H	-1.197027	1.227579	0.542578
45	H	3.444578	7.36417	0.654983
46	H	3.92458	7.457628	-1.02446
47	H	0.966022	0.064815	1.152899
48	H	1.476239	0.16615	-0.523246
49	H	-0.58969	18.271135	-0.019193
50	H	0.880329	17.628801	-0.760243
51	H	0.685466	17.58889	0.995077
52	H	6.088342	8.574524	-0.31464
53	H	5.54227	8.521334	1.353016
54	H	-1.038372	16.02297	-1.012278

55	H	-1.244877	15.983398	0.737835
56	H	3.552664	9.941923	0.7223
57	H	4.152374	10.021516	-0.927759
58	H	1.0432	15.009934	0.996987
59	H	1.277968	15.079562	-0.744724
60	H	6.261814	11.120224	-0.114064
61	H	5.663909	11.028353	1.535737
62	H	-1.102126	13.654556	-0.375298
63	H	3.651678	12.397169	0.359939
64	H	-0.76011	11.297184	-1.099182
65	H	-1.157247	11.290789	0.608716
66	H	3.496715	14.593277	0.193774
67	H	4.25862	14.7441	-1.382324
68	H	0.864404	9.913867	1.095549
69	H	1.332882	9.972906	-0.589218
70	H	6.113654	16.081095	-0.365819
71	H	5.332279	15.991061	1.197147
72	H	-0.777868	8.798572	-1.239599
73	H	-1.284895	8.751408	0.439852
74	H	3.825611	-0.275937	0.603476
75	H	4.057985	-0.157572	-1.129967
76	H	4.098895	17.306051	-1.297354
77	H	4.788724	18.169321	0.081755
78	H	3.318916	17.210835	0.286626
79	H	0.684303	7.322415	1.010952
80	H	1.236679	7.404975	-0.657194
81	H	5.985452	1.403774	-0.770767
82	H	5.757562	1.271385	0.971888
83	H	-1.423117	6.187243	0.27466
84	H	-0.911232	6.323593	-1.401669
85	H	3.706164	2.395507	-1.013277
86	H	3.431623	2.210987	0.713981
87	H	-0.998292	-1.355849	0.476067
88	H	0.526434	-2.093296	-0.034033
89	H	-0.490803	-1.252406	-1.2117
90	H	6.123558	-1.281727	0.851036
91	H	6.359356	-1.161421	-0.896902
92	H	5.119726	-2.237963	-0.244199

Table S2. Computational and experimental vibrational frequencies and the assignments of main bands presented in Fig. 2.

Computational frequency (cm^{-1})	**Experimental frequency (cm^{-1})**	**Assignment**
1160	1126	C-C stretching (*trans*)
1105	1080	C-C stretching (*gauche*)
1090	1060	C-C stretching (*trans*)
113	100	CH_2 lateral motion
110		C=O and N-H stretching
107		
72	60	Backbone rotational motion
63		