

Supplementary Information :

Estimation of Dielectric Constant of Polymer Melt by Machine Learning Considering with Higher-order Structure

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Table S1: Polymer sample condition

Polymer type label	Sample No.	Composition	Dielectric Constant
0	1	AN 50% BD 50%	1.054
0	2	AN 45% BD 55%	1.188
0	3	AN 40% BD 60%	1.177
0	4	AN 35% BD 65%	1.192
0	5	AN 30% BD 70%	1.170
0	6	AN 25% BD 75%	1.144
0	7	AN 20% BD 80%	1.147
0	8	AN 15% BD 85%	1.118
0	9	AN 10% BD 90%	1.076
0	10	AN 5% BD 95%	1.049
0	11	AN 95% BD 5%	1.013
0	12	AN 90% BD 10%	1.075
0	13	AN 85% BD 15%	1.160
0	14	AN 80% BD 20%	1.151
0	15	AN 75% BD 25%	1.190
0	16	AN 70% BD 30%	1.225
0	17	AN 65% BD 35%	1.215
0	18	AN 60% BD 40%	1.249
0	19	AN 55% BD 45%	1.228
1	20	EA 0% BA 0% BEA 100%	1.015
1	21	EA 0% BA 10% BEA 90%	1.017
1	22	EA 0% BA 20% BEA 80%	1.006
1	23	EA 0% BA 30% BEA 70%	1.012
1	24	EA 0% BA 40% BEA 60%	1.010
1	25	EA 0% BA 50% BEA 50%	1.018
1	26	EA 0% BA 60% BEA 40%	1.012
1	27	EA 0% BA 70% BEA 30%	1.006
1	28	EA 0% BA 80% BEA 20%	1.018
1	29	EA 0% BA 90% BEA 10%	1.016
1	30	EA 0% BA 100% BEA 0%	1.006
1	31	EA 10% BA 0% BEA 90%	1.032
1	32	EA 10% BA 10% BEA 80%	1.025
1	33	EA 10% BA 20% BEA 70%	1.006
1	34	EA 10% BA 30% BEA 60%	1.014
1	35	EA 10% BA 40% BEA 50%	1.022
1	36	EA 10% BA 50% BEA 40%	1.011
1	37	EA 10% BA 60% BEA 30%	1.008

Polymer type label	Sample No.	Composition	Dielectric Constant
1	38	EA 10% BA 70% BEA 20%	1.016
1	39	EA 10% BA 80% BEA 10%	1.007
1	40	EA 10% BA 90% BEA 0%	1.002
1	41	EA 20% BA 0% BEA 80%	1.030
1	42	EA 20% BA 10% BEA 70%	1.007
1	43	EA 20% BA 20% BEA 60%	1.010
1	44	EA 20% BA 30% BEA 50%	1.015
1	45	EA 20% BA 40% BEA 40%	1.027
1	46	EA 20% BA 50% BEA 30%	1.030
1	47	EA 20% BA 60% BEA 20%	1.013
1	48	EA 20% BA 70% BEA 10%	1.006
1	49	EA 20% BA 80% BEA 0%	1.023
1	50	EA 30% BA 0% BEA 70%	1.038
1	51	EA 30% BA 10% BEA 60%	1.006
1	52	EA 30% BA 20% BEA 50%	1.024
1	53	EA 30% BA 30% BEA 40%	1.026
1	54	EA 30% BA 40% BEA 30%	1.023
1	55	EA 30% BA 50% BEA 20%	1.015
1	56	EA 30% BA 60% BEA 10%	1.030
1	57	EA 30% BA 70% BEA 0%	1.025
1	58	EA 40% BA 0% BEA 60%	1.031
1	59	EA 40% BA 10% BEA 50%	1.023
1	60	EA 40% BA 20% BEA 40%	1.036
1	61	EA 40% BA 30% BEA 30%	1.044
1	62	EA 40% BA 40% BEA 20%	1.039
1	63	EA 40% BA 50% BEA 10%	1.017
1	64	EA 40% BA 60% BEA 0%	1.046
1	65	EA 50% BA 0% BEA 50%	1.050
1	66	EA 50% BA 10% BEA 40%	1.052
1	67	EA 50% BA 20% BEA 30%	1.042
1	68	EA 50% BA 30% BEA 20%	1.021
1	69	EA 50% BA 40% BEA 10%	1.020
1	70	EA 50% BA 50% BEA 0%	1.029
1	71	EA 60% BA 0% BEA 40%	1.028
1	72	EA 60% BA 10% BEA 30%	1.028
1	73	EA 60% BA 20% BEA 20%	1.035
1	74	EA 60% BA 30% BEA 10%	1.048
1	75	EA 60% BA 40% BEA 0%	1.039
1	76	EA 70% BA 0% BEA 30%	1.044
1	77	EA 70% BA 10% BEA 20%	1.041
1	78	EA 70% BA 0% BEA 30%	1.044
1	79	EA 80% BA 0% BEA 20%	1.048
1	80	EA 80% BA 10% BEA 10%	1.086
1	81	EA 80% BA 20% BEA 0%	1.039
1	82	EA 90% BA 0% BEA 10%	1.045
1	83	EA 90% BA 10% BEA 0%	1.042
2	84	VF 20% HF 50% TF 30%	1.067
2	85	VF 20% HF 60% TF 20%	1.047
2	86	VF 20% HF 70% TF 10%	1.036
2	87	VF 20% HF 80% TF 0%	1.053
2	88	VF 30% HF 10% TF 60%	1.148
2	89	VF 30% HF 20% TF 50%	1.097
2	90	VF 30% HF 30% TF 40%	1.119
2	91	VF 30% HF 40% TF 30%	1.097
2	92	VF 30% HF 50% TF 20%	1.069
2	93	VF 30% HF 60% TF 10%	1.029
2	94	VF 30% HF 70% TF 0%	1.040
2	95	VF 40% HF 10% TF 50%	1.144
2	96	VF 40% HF 20% TF 40%	1.147
2	97	VF 40% HF 30% TF 30%	1.101
2	98	VF 40% HF 40% TF 20%	1.075
2	99	VF 40% HF 50% TF 10%	1.078

Polymer type label	Sample No.	Composition	Dielectric Constant
2	100	VF 40% HF 60% TF 0%	1.027
2	101	VF 50% HF 10% TF 40%	1.204
2	102	VF 50% HF 20% TF 30%	1.162
2	103	VF 50% HF 30% TF 20%	1.081
2	104	VF 50% HF 40% TF 10%	1.063
2	105	VF 50% HF 50% TF 0%	1.034
2	106	VF 60% HF 10% TF 30%	1.119
2	107	VF 60% HF 20% TF 20%	1.104
2	108	VF 60% HF 30% TF 10%	1.087
2	109	VF 60% HF 40% TF 0%	1.061
2	110	VF 70% HF 10% TF 20%	1.121
2	111	VF 70% HF 20% TF 10%	1.067
2	112	VF 70% HF 30% TF 0%	1.089
2	113	VF 80% HF 10% TF 10%	1.081
2	114	VF 80% HF 20% TF 0%	1.063
2	115	VF 90% HF 10% TF 0%	1.052
2	116	VF 10% HF 10% TF 80%	1.126
2	117	VF 10% HF 20% TF 70%	1.082
2	118	VF 10% HF 30% TF 60%	1.071
2	119	VF 10% HF 40% TF 50%	1.054
2	120	VF 10% HF 50% TF 40%	1.055
2	121	VF 10% HF 60% TF 30%	1.030
2	122	VF 10% HF 70% TF 20%	1.014
2	123	VF 10% HF 80% TF 10%	1.006
2	124	VF 10% HF 90% TF 0%	1.039
2	125	VF 20% HF 10% TF 70%	1.116
2	126	VF 20% HF 20% TF 60%	1.027
2	127	VF 20% HF 30% TF 50%	1.082
2	128	VF 20% HF 40% TF 400%	1.088
3	129	DMS 95% MVS 5% MFS 0%	1.091
3	130	DMS 90% MVS 5% MFS 5%	1.145
3	131	DMS 85% MVS 5% MFS 10%	1.228
3	132	DMS 80% MVS 5% MFS 15%	1.171
3	133	DMS 75% MVS 5% MFS 30%	1.176
3	134	DMS 70% MVS 5% MFS 25%	1.146
3	135	DMS 65% MVS 5% MFS 30%	1.418
3	136	DMS 60% MVS 5% MFS 35%	1.299
3	137	DMS 55% MVS 5% MFS 40%	1.231
3	138	DMS 50% MVS 5% MFS 45%	1.260
3	139	DMS 45% MVS 5% MFS 50%	1.184
3	140	DMS 40% MVS 5% MFS 55%	1.169
3	141	DMS 35% MVS 5% MFS 60%	1.085
3	142	DMS 30% MVS 5% MFS 65%	1.081
3	143	DMS 25% MVS 5% MFS 70%	1.065
3	144	DMS 20% MVS 5% MFS 75%	1.107
3	145	DMS 15% MVS 5% MFS 80%	1.069
3	146	DMS 10% MVS 5% MFS 85%	1.059
3	147	DMS 5% MVS 5% MFS 90%	1.111
4	148	76-112-63-71	1.043
4	149	96-102-137-9	1.145
4	150	118-124-68-131	1.039
4	151	22-112-119-125	1.102
4	152	131-31-133-105	1.119
4	153	72-94-17-82	1.058
4	154	41-133-116-92	1.022
4	155	47-99-60-8	1.072
4	156	140-17-128-9	1.061
4	157	20-104-77-38	1.198
4	158	36-49-135-42	1.047
4	159	7-130-63-102	1.088
4	160	76-29-48-34	1.091
4	161	112-31-75-10	1.01

Polymer type label	Sample No.	Composition	Dielectric Constant
4	162	18-61-136-90	1.026
4	163	73-69-4-39	1.153
4	164	9-81-80-148	1.036
4	165	120-74-17-63	1.107
4	166	98-91-140-47	1.045
4	167	26-29-54-33	1.052
4	168	83-24-7-145	1.012
4	169	65-11-9-113	1.08
4	170	125-60-109-77	1.144
4	171	83-60-4-67	1.027
4	172	2-90-148-34	1.065
4	173	87-132-87-21	1.049
4	174	5-27-102-7	1.12
4	175	60-3-67-89	1.138
4	176	30-2-70-45	1.018
4	177	88-58-17-26	1.037
4	178	22-110-143-49	1.014
4	179	2-91-17-11	1.042
4	180	110-88-143-104	1.101
4	181	61-52-142-4	1.083
4	182	133-32-119-118	1.099
4	183	127-38-67-88	1.09
4	184	137-42-59-134	1.039
4	185	38-135-132-120	1.092
4	186	16-84-79-21	1.084
4	187	122-91-106-108	1.034
4	188	52-51-28-59	1.118
4	189	113-114-65-125	1.016
4	190	117-41-127-88	1.1
4	191	94-105-145-36	1.042
4	192	118-100-61-55	1.047
4	193	125-105-14-99	1.051
4	194	123-92-52-51	1.124
4	195	41-102-99-76	1.091
4	196	53-148-83-81	1.037
4	197	109-116-65-60	1.045
4	198	148-147-3-33	1.05
4	199	123-146-75-73	1.055
4	200	30-9-119-13	1.06
4	201	15-40-105-101	1.139
4	202	57-47-81-76	1.053
4	203	96-52-127-141	1.033
4	204	58-113-106-135	1.031
4	205	112-45-137-147	1.04
4	206	20-27-43-71	1.075
4	207	82-10-148-25	1.009
4	208	139-25-32-19	1.081
4	209	60-128-100-114	1.112
4	210	17-100-45-54	1.045
4	211	69-60-58-21	1.05
4	212	13-34-5-58	1.021
4	213	132-65-51-11	1.1
4	214	35-121-97-39	1.049
4	215	25-128-72-110	1.069
4	216	72-110-108-60	1.033
4	217	37-49-102-72	1.018
4	218	125-59-51-88	1.013
4	219	124-12-29-135	1.061
4	220	9-144-112-26	1.057
4	221	138-135-97-51	1.035
4	222	31-33-63-88	1.149
4	223	61-22-69-29	1.017

Polymer type label	Sample No.	Composition	Dielectric Constant
4	224	83-59-135-55	1.02
4	225	93-119-27-58	1.153
4	226	127-121-30-40	1.026
4	227	49-84-46-93	1.026
4	228	78-66-121-65	1.023

Polymer type label: 0 is NBR, 1 is ACM, 2 is FKM, 3 is VMQ and 4 is Blend polymer.
% means mol% in this table.

AN is Acrylonitrile and BD is Butadiene in label 0.

EA is Ethyl acrylate, BA is Butyl acrylate and BEA is 2-Methoxyethyl acrylate in label No.1.

VF is Vinylidene fluoride, HF is Hexafluoropropylene and TF is Tetrafluoroethylene in label No.2.

DMS is Didimethylsiloxane, MVS is Methyl vinyl siloxane and MFS is Methylphenylsiloxane in label No.3.

In the blend polymer of label No.4, a total of 4 types of monomers corresponding to the sample number are randomly blended.

Table S2: The sample of fingerprints descriptor of ECFP6

[illegible]

Table S3: The sample of fingerprints descriptor of persistent diagram vector

Sample No.	Polymer	Persistent diagram vector (Original 2080 vector)																																	
1	NBR	0	0	...	0	0.0024	0	0	0	0	0.0131	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
2	NBR	0	0	...	0	0.0034	0	0	0	0	0.0131	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3	NBR	0	0	...	0	0.0034	0	0	0	0	0.0168	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
4	NBR	0	0	...	0	0.0034	0	0	0	0	0.0140	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
5	NBR	0	0	...	0	0.0027	0	0	0	0	0.02197	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
⋮				...								...																							
20	ACM	0	0	...	0	0.0076	0	0	0	0	0.0937	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
21	ACM	0	0	...	0	0.0046	0	0	0	0	0.0827	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
22	ACM	0	0	...	0	0.0067	0	0	0	0	0.0745	...	0	0	0	0	0	0	0	0	0	0	0	0.2189	0	0	0	0	0	0	0	0	0	0.0006	0
23	ACM	0	0	...	0	0.0095	0	0	0	0	0.0623	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
24	ACM	0	0	...	0	0.0095	0	0	0	0	0.0641	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0003	0
⋮				...								...																							
84	FKM	0	0	...	0	0	0	0	0	0	0.0104	...	0	0	0	0	0	0	0	0	0	0	0.1043	0.0658	0	0.0195	0	0	0.0012	0	0	0	0	0	
85	FKM	0	0	...	0	0	0	0	0	0	0.0134	...	0	0.9826	0	0	0	0	0	0.4853	0	0	0	0	0.0638	0.0381	0	0	0.0098	0.0021	0	0	0	0	
86	FKM	0	0	...	0	0	0	0	0	0	0.0153	...	2.115	0	0	0	0	0	0.9706	0	0	0	0	0	0	0	0.0195	0	0	0.0021	0	0	0	0	
87	FKM	0	0	...	0	0	0	0	0	0	0.0140	...	0	0	0	0	0	0.3858	0	0	0.6971	0	0	0.1550	0	0.0381	0.0586	0.0082	0.0049	0.0034	0	0	0	0	
88	FKM	0	0	...	0	0	0	0	0	0	0.0067	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0195	0.0082	0	0.0012	0	0	0	0	
⋮				...								...																							
129	VMQ	0	0	...	0	0	0	0	0	0	0.0253	...	0	0	0	0	0	0	0.3858	0	0	0	0	0	0	0	0	0	0.0024	0.0012	0	0	0	0	
130	VMQ	0	0	...	0	0	0	0	0	0	0.0333	...	0	0	0	0	0	0	0	0	0	0	0.1550	0	0	0	0	0	0.0003	0	0	0	0	0	
131	VMQ	0	0	...	0	0	0	0	0	0	0.0262	...	0	0	0	0	0	0	0	0	0	0	0	0	0.0658	0	0	0.0024	0.0006	0	0	0	0	0	
132	VMQ	0	0	...	0	0	0	0	0	0	0.0189	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0.1144	0	0	0.0006	0	0	0	0	0	
133	VMQ	0	0	...	0	0	0	0	0	0	0.0259	...	0	0	0	0	0	0	0	0	0	0	0	0	0.0658	0	0	0.0003	0	0	0	0	0	0	
⋮				...								...																							
148	Blend	0	0	...	0	0.0067	0	0	0	0	0.0183	...	0	0	0	0	0	0	0	0	0	0	0	0	0.1043	0	0	0.0195	0	0	0.0009	0	0	0	
149	Blend	0	0	...	0	0.0018	0	0	0	0	0.014	...	1.125	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0009	0	
150	Blend	0	0	...	0	0.0055	0	0	0	0	0.0208	...	0	0	0	0	0	0	0.3858	0	0	0	0	0	0	0.10430	0	0	0.0082	0.0049	0	0	0	0	
151	Blend	0	0	...	0	0.0018	0	0	0	0	0.0116	...	0	1.059	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0195	0	0	0.0009	0	0	
152	Blend	0	0	...	0	0.0021	0	0	0	0	0.0177	...	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0195	0	0.0024	0.0003	0	0	0	0

Table S4: The sample of Cell image and Persistent diagram(PD)

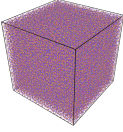
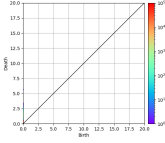
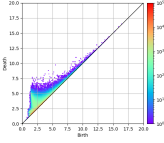
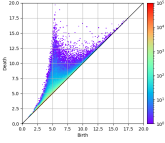
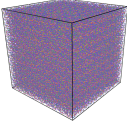
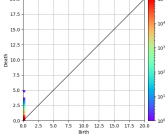
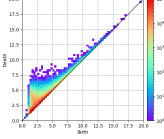
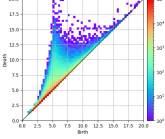
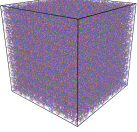
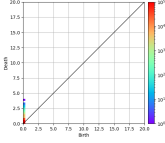
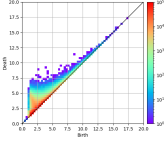
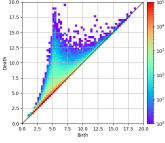
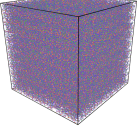
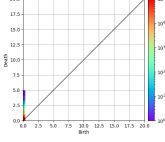
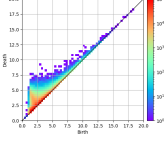
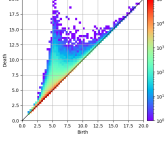
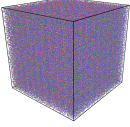
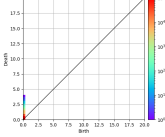
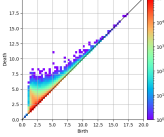
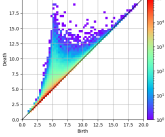
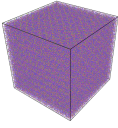
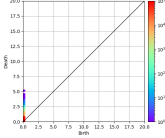
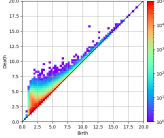
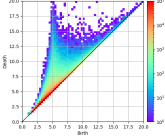
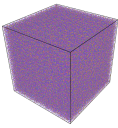
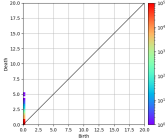
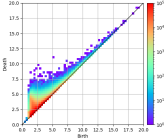
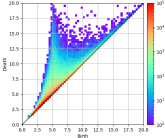
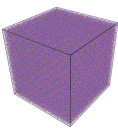
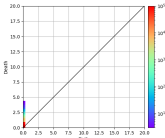
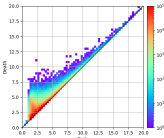
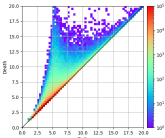
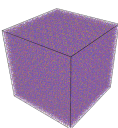
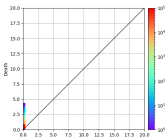
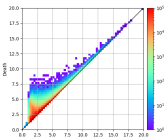
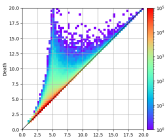
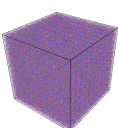
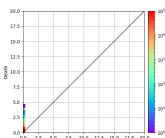
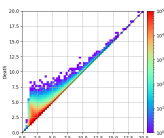
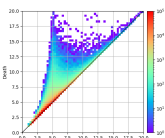
Sample No.	Polymer	Cell image	0th PD	1st PD	2nd PD
1	NBR				
2	NBR				
3	NBR				
4	NBR				
5	NBR				
⋮					
20	ACM				
21	ACM				
22	ACM				
23	ACM				
24	ACM				

Table S5: The sample of Cell image and Persistent diagram(PD)

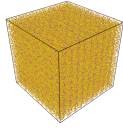
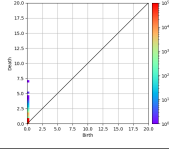
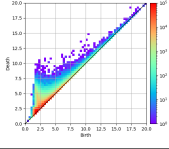
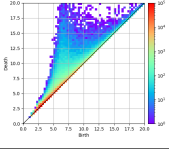
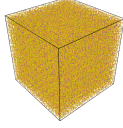
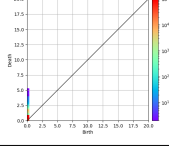
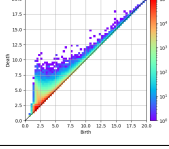
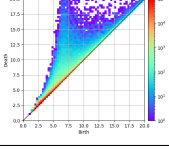
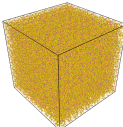
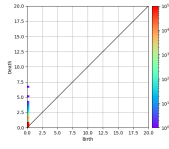
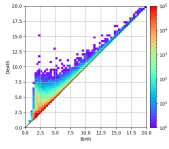
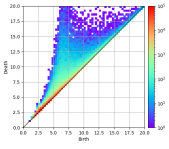
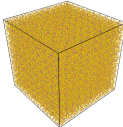
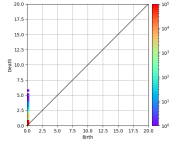
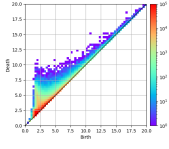
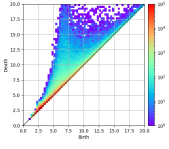
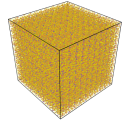
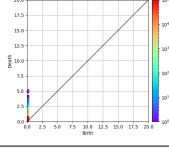
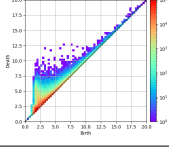
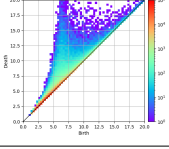
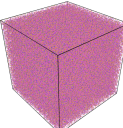
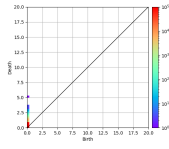
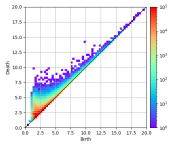
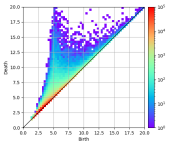
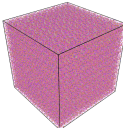
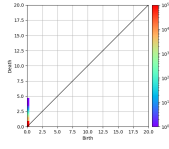
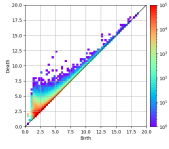
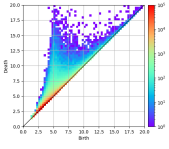
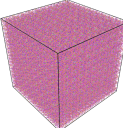
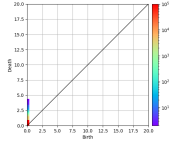
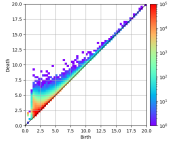
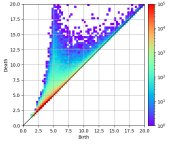
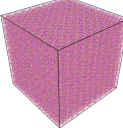
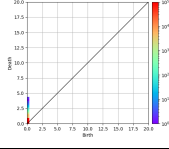
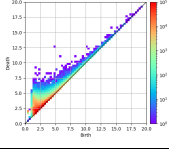
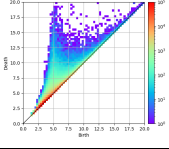
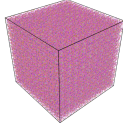
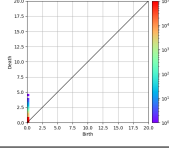
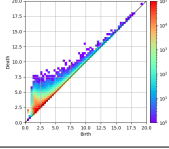
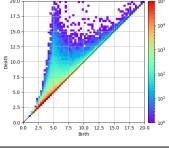
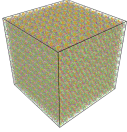
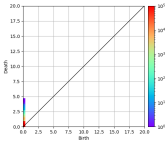
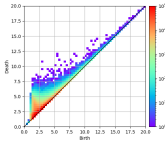
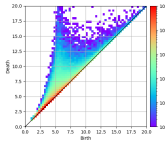
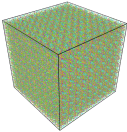
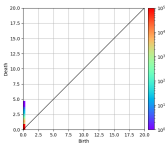
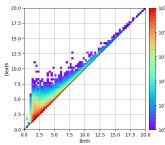
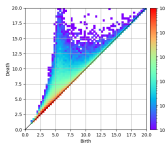
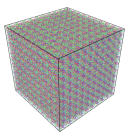
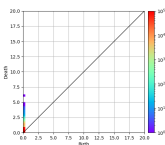
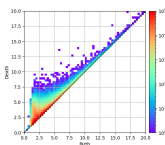
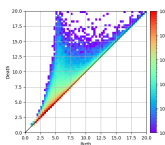
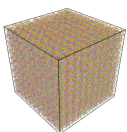
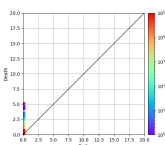
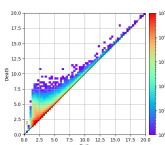
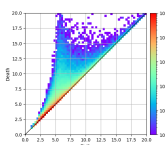
Sample No.	Polymer	Cell image	0th PD	1st PD	2nd PD
84	FKM				
85	FKM				
86	FKM				
87	FKM				
88	FKM				
⋮					
129	VMQ				
130	VMQ				
131	VMQ				
132	VMQ				
133	VMQ				

Table S6: The sample of Cell image and Persistent diagram(PD)

Sample No.	Polymer	Cell image	0th PD	1st PD	2nd PD
148	Blend				
149	Blend				
150	Blend				
151	Blend				
152	Blend	