

Supplementary Material for

Combining *ab initio* and *ab initio* molecular dynamics simulations to predict the complex refractive index of organic polymers

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Table S1 Polarizability and refractive index of PVC

n	α_{ORCA} (bohr ³)	N ($\times 10^{28} \text{ m}^{-3}$)	n_r	α_{linear} (bohr ³)	$n_{r_{\text{linear}}}$	Relative difference	α_{PPFS} (bohr ³)	$n_{r_{\text{PPFS}}}$	Relative difference
1	37.7160	1.3137E+00	1.5272	34.1023	1.4676	5.96E-02	37.7160	1.5266	6.43E-04
2	72.7963	6.6724E-01	1.5149	70.5563	1.4956	1.93E-02	72.7963	1.5143	6.25E-04
3	107.5668	4.4719E-01	1.5090	107.0103	1.5053	3.73E-03	107.5668	1.5084	6.15E-04
4	143.8035	3.3628E-01	1.5122	143.4643	1.5102	2.05E-03	141.2306	1.5008	1.14E-02
5	179.6527	2.6946E-01	1.5128	179.9183	1.5131	2.78E-04	177.7549	1.5058	7.03E-03
10	358.9473	1.3516E-01	1.5142	362.1883	1.5191	4.90E-03	360.3766	1.5160	1.81E-03
20	724.7406	6.7690E-02	1.5210	726.7283	1.5221	1.07E-03	725.6199	1.5211	1.19E-04
30	1084.6637	4.5151E-02	1.5200	1091.2683	1.5231	3.14E-03	1090.8632	1.5229	2.91E-03
40	1456.4855	3.3872E-02	1.5245	1455.8083	1.5236	9.29E-04	1456.1065	1.5237	8.01E-04
50	1825.0084	2.7102E-02	1.5262	1820.3483	1.5239	2.24E-03	1821.3498	1.5243	1.90E-03
100	-	-	-	3643.0483	1.5245	-	3647.5664	1.5253	-
200	-	-	-	7288.4483	1.5248	-	7299.9996	1.5258	-
500	-	-	-	18224.6483	1.5250	-	18257.2991	1.5261	-
1000	-	-	-	36451.6483	1.5251	-	36519.4649	1.5262	-
2000	-	-	-	72905.6483	1.5251	-	73043.7965	1.5263	-

Table S2 Polarizability and refractive index of PVA

n	α_{ORCA} (bohr ³)	N ($\times 10^{28} \text{ m}^{-3}$)	n_r	α_{linear} (bohr ³)	$n_{r_{\text{linear}}}$	Relative difference	α_{PPFS} (bohr ³)	$n_{r_{\text{PPFS}}}$	Relative difference
1	31.1022	1.6680E+00	1.5565	30.8581	1.5512	5.28E-03	31.1023	1.5565	2.41E-06
2	58.1392	8.5267E-01	1.5269	59.1841	1.5383	1.14E-02	58.1392	1.5269	1.25E-07
3	86.1717	5.7273E-01	1.5241	87.5101	1.5339	9.75E-03	86.1717	1.5241	1.21E-07
4	113.5730	4.3114E-01	1.5192	115.8361	1.5316	1.24E-02	116.5584	1.5356	1.64E-02
5	142.6223	3.4570E-01	1.5235	144.1621	1.5303	6.76E-03	144.8626	1.5334	9.85E-03
10	290.6891	1.7364E-01	1.5384	285.7921	1.5276	1.08E-02	286.3835	1.5289	9.54E-03
20	571.7931	8.7018E-02	1.5293	569.0521	1.5262	3.03E-03	569.4253	1.5266	2.62E-03

30	852.6270	5.8056E-02	1.5260	852.3121	1.5258	2.32E-04	852.4671	1.5259	1.18E-04
40	1134.6769	4.3559E-02	1.5250	1135.5721	1.5255	4.95E-04	1135.5089	1.5255	4.60E-04
50	1417.7750	3.4855E-02	1.5249	1418.8321	1.5254	4.67E-04	1418.5507	1.5253	3.43E-04
100	-	-	-	2835.1321	1.5251	-	2833.7597	1.5248	-
200	-	-	-	5667.7321	1.5250	-	5664.1776	1.5246	-
500	-	-	-	14165.5321	1.5249	-	14155.4314	1.5245	-
1000	-	-	-	28328.5321	1.5249	-	28307.5212	1.5244	-
2000	-	-	-	56654.5321	1.5249	-	56611.7006	1.5244	-

Table S3 Polarizability and refractive index of PLA

n	α_{ORCA} (bohr ³)	N ($\times 10^{28} \text{ m}^{-3}$)	n_r	α_{linear} (bohr ³)	$n_{r_{\text{linear}}}$	Relative difference	α_{PPFS} (bohr ³)	$n_{r_{\text{PPFS}}}$	Relative difference
1	43.9342	1.0269E+00	1.4715	42.9273	1.4589	1.25E-02	43.9342	1.4715	1.95E-07
2	84.3933	5.2052E-01	1.4571	83.5613	1.4519	5.21E-03	84.3933	1.4571	1.41E-07
3	125.4478	3.4862E-01	1.4547	124.1953	1.4495	5.25E-03	125.4478	1.4547	1.41E-09
4	163.4898	2.6206E-01	1.4441	164.8293	1.4483	4.20E-03	163.6471	1.4446	4.93E-04
5	205.8237	2.0994E-01	1.4485	205.4633	1.4476	9.06E-04	204.3275	1.4447	3.76E-03
10	407.4819	1.0527E-01	1.4447	408.6333	1.4461	1.45E-03	407.7298	1.4450	3.12E-04
20	817.4324	5.2706E-02	1.4469	814.9733	1.4454	1.55E-03	814.5343	1.4451	1.83E-03
30	1211.6159	3.5154E-02	1.4411	1221.3133	1.4452	4.07E-03	1221.3388	1.4452	4.08E-03
40	1633.8771	2.6372E-02	1.4470	1627.6533	1.4450	1.96E-03	1628.1433	1.4452	1.81E-03
100	-	-	-	4065.6933	1.4447	-	4068.9703	1.4452	-
200	-	-	-	8129.0933	1.4447	-	8137.0154	1.4452	-
500	-	-	-	20319.2933	1.4447	-	20341.1505	1.4452	-
1000	-	-	-	40636.2933	1.4447	-	40681.3756	1.4452	-
2000	-	-	-	81270.2933	1.4447	-	81361.8260	1.4452	-