Supplementary Information for

Anharmonicity-induced thermal rectification of a single diblock molecule inspired by the Aviram–Ratner diode

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S1. Computational details and structure of the molecular junctions

All the atomic structures and force constant matrices were obtained using density functional theory with the functional PBEsol exchange-correlation (XC). We adopted the single zeta plus polarization (SZP) level basis set and performed practical calculations using the SIESTA program package[1]. The left/right electrodes of a molecular junction consist of six atomic layers of 3×3 Au(111), where the bridge site is considered as the adsorption site of the molecule. All atomic positions were relaxed to determine the energetically optimized structure, while the lattice constant was fixed. The frozen phonon approximation was applied for force constant calculations. The resulting atomic structures of C_2Ph_2, CHO_2PhPy, and $(CHO_2)_2Ph_2$ molecular junctions are shown in Figure S1-1.

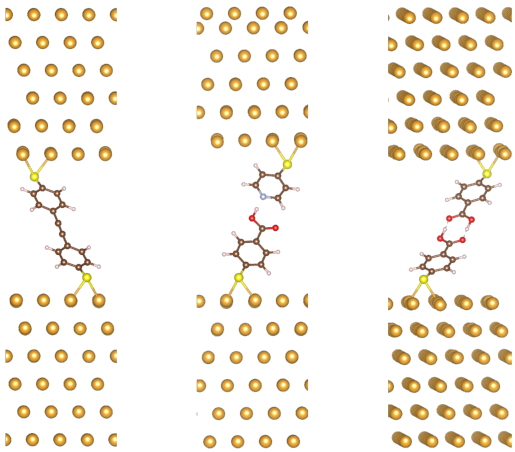

Figure S1-1. Structures of the molecular junctions. The left, middle, and right panels show the C_2Ph_2, CHO_2PhPy, and $(CHO_2)_2Ph_2$ junctions.

All of the atomic coordinates are given below as xyz format.

C_2Ph_2

```
CRYSTAL
PRIMVEC
   8.6520    0.0000    0.0000
   4.3260    7.4929    0.0000
   0.0000    0.0000   38.464
PRIMCOORD
        123 1
   79         0.0000       0.0000       0.0000
   79         2.8840       0.0000       0.0000
   79         5.7680       0.0000       0.0000
   79         1.4420       2.4976       0.0000
   79         4.3260       2.4976       0.0000
   79         7.2100       2.4976       0.0000
   79         2.8840       4.9952       0.0000
   79         5.7680       4.9952       0.0000
   79         8.6520       4.9952       0.0000
   79         0.0025       1.5958       2.5246
   79         2.8860       1.5966       2.5220
   79         5.7711       1.5964       2.5222
   79         1.4451       4.0925       2.5186
   79         4.3285       4.0929       2.5175
   79         7.2119       4.0924       2.5186
   79         2.8863       6.5915       2.5206
   79         5.7708       6.5915       2.5205
   79         8.6545       6.5918       2.5205
   79         1.4492       0.6985       5.0378
   79         4.3315       0.7000       5.0446
   79         7.2135       0.6983       5.0381
   79         2.8920       3.1924       5.0439
   79         5.7709       3.1925       5.0439
   79         8.6573       3.1966       5.0373
   79         4.3314       5.6896       5.0288
   79         7.2165       5.6934       5.0329
   79        10.0982       5.6931       5.0332
   79         0.0076      -0.1954       7.5362
   79         2.8924      -0.1948       7.5601
   79         5.7750      -0.1950       7.5607
   79         1.4514       2.2977       7.5562
   79         4.3337       2.2849       7.5964
   79         7.2159       2.2979       7.5563
   79         2.8900       4.7975       7.5383
   79         5.7769       4.7977       7.5382
   79         8.6595       4.7985       7.5513
   79         0.0087       1.4137      10.0724
   79         2.8759       1.4075      10.1217
   79         5.7934       1.4076      10.1219
   79         1.4554       3.9147      10.0405
   79         4.3345       3.9017      10.0176
   79         7.2138       3.9147      10.0406
   79         2.8930       6.4193      10.0429
   79         5.7762       6.4190      10.0424
   79         8.6605       6.4174      10.0522
   79         1.5009       0.5836      12.6515
   79         4.3347       0.5748      12.6362
   79         7.1682       0.5854      12.6530
   79         2.8962       3.0851      12.6284
```

79	5.7731	3.0856	12.6280
79	8.6610	3.0918	12.5499
79	4.3347	5.5327	12.4878
79	7.2245	5.5631	12.5868
79	10.0978	5.5634	12.5865
16	0.0093	0.2442	14.7023
6	0.0216	1.7617	15.6233
1	2.2035	1.8761	15.6839
1	-2.1578	1.9269	15.6710
6	1.2536	2.2962	16.0768
6	-1.2005	2.3249	16.0693
6	1.2616	3.3154	17.0308
6	-1.1899	3.3444	17.0230
1	2.2204	3.7190	17.4124
1	-2.1416	3.7708	17.3989
6	0.0403	3.8246	17.5506
6	0.0462	4.7676	18.6178
6	0.0460	5.5270	19.5933
6	0.0390	6.4269	20.6965
1	2.2186	6.4868	20.8727
1	-2.1435	6.5140	20.8120
6	1.2602	6.8809	21.2658
6	-1.1916	6.8962	21.2320
6	1.2532	7.8300	22.2897
6	-1.2011	7.8449	22.2559
1	2.2029	8.2040	22.7284
1	-2.1580	8.2305	22.6683
6	0.0224	8.3515	22.7595
16	0.0140	9.8013	23.7816
79	0.0116	1.8839	25.8247
79	2.8449	1.8720	25.8111
79	5.8298	1.8728	25.8120
79	1.4479	4.3883	25.8830
79	4.3371	4.4261	25.9941
79	7.2270	4.3886	25.8832
79	2.8973	6.8684	25.8336
79	5.7773	6.8681	25.8325
79	8.6633	6.8621	25.9077
79	1.4695	1.0616	28.3395
79	4.3362	1.0561	28.3917
79	7.2029	1.0617	28.3392
79	2.8944	3.5430	28.4291
79	5.7787	3.5430	28.4292
79	8.6624	3.5443	28.4142
79	4.3363	6.0618	28.4500
79	7.2161	6.0479	28.4236
79	10.1083	6.0477	28.4239
79	0.0088	0.2003	30.8647
79	2.8909	0.1866	30.9059
79	5.7791	0.1866	30.9061
79	1.4496	2.6789	30.9066
79	4.3349	2.6796	30.9313
79	7.2202	2.6789	30.9068
79	2.8914	5.1799	30.9289
79	5.7785	5.1798	30.9289
79	8.6608	5.1792	30.9149
79	0.0067	1.7891	33.4207
79	2.8889	1.7907	33.4265
79	5.7765	1.7908	33.4270
79	1.4476	4.2891	33.4334
79	4.3328	4.2926	33.4383
79	7.2181	4.2892	33.4335

79	2.8931	6.7897	33.4204
79	5.7722	6.7897	33.4200
79	8.6588	6.7858	33.4271
79	1.4457	0.8959	35.9424
79	4.3292	0.8969	35.9392
79	7.2125	0.8958	35.9426
79	2.8870	3.3936	35.9444
79	5.7715	3.3937	35.9446
79	8.6552	3.3928	35.9457
79	4.3291	5.8927	35.9473
79	7.2124	5.8932	35.9455
79	10.0977	5.8930	35.9458

$(CHO_2)PhPy$

CRYSTAL
PRIMVEC
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4.3260 7.4929 0.0000
0.0000 0.0000 39.68
PRIMCOORD
125 1

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79	2.8840	0.0000	0.0000
79	5.7680	0.0000	0.0000
79	1.4420	2.4976	0.0000
79	4.3260	2.4976	0.0000
79	7.2100	2.4976	0.0000
79	2.8840	4.9952	0.0000
79	5.7680	4.9952	0.0000
79	8.6520	4.9952	0.0000
79	0.0061	1.6024	2.5278
79	2.8896	1.6034	2.5256
79	5.7744	1.6035	2.5271
79	1.4493	4.0992	2.5221
79	4.3325	4.0992	2.5221
79	7.2154	4.0988	2.5228
79	2.8899	6.5983	2.5239
79	5.7743	6.5983	2.5234
79	8.6581	6.5988	2.5218
79	1.4532	0.7150	5.0447
79	4.3352	0.7170	5.0508
79	7.2173	0.7155	5.0452
79	2.8961	3.2089	5.0513
79	5.7745	3.2095	5.0541
79	8.6614	3.2119	5.0432
79	4.3351	5.7066	5.0355
79	7.2204	5.7100	5.0373
79	10.1020	5.7099	5.0370
79	0.0107	-0.1591	7.5469
79	2.8948	-0.1578	7.5699
79	5.7781	-0.1580	7.5679
79	1.4545	2.3321	7.5692
79	4.3355	2.3206	7.6142
79	7.2187	2.3326	7.5707
79	2.8933	4.8337	7.5459
79	5.7802	4.8344	7.5479
79	8.6625	4.8340	7.5538
79	0.0121	1.4787	10.0997
79	2.8742	1.4726	10.1486

79	5.8000	1.4750	10.1433
79	1.4583	3.9830	10.0438
79	4.3389	3.9693	10.0292
79	7.2186	3.9827	10.0470
79	2.8979	6.4887	10.0555
79	5.7795	6.4892	10.0570
79	8.6660	6.4867	10.0552
79	1.5093	0.7055	12.7155
79	4.3463	0.6816	12.6455
79	7.1833	0.6991	12.7117
79	2.9078	3.1964	12.6201
79	5.7836	3.1940	12.6369
79	8.6684	3.2043	12.5559
79	4.3444	5.6445	12.4994
79	7.2312	5.6780	12.5869
79	10.1088	5.6760	12.5955
16	0.0402	0.3193	14.7515
6	-0.0012	1.7052	15.8724
1	1.7702	2.7510	15.1129
1	-1.7697	0.8513	16.8442
6	0.9832	2.7223	15.9025
6	-0.9991	1.6497	16.8764
6	0.9823	3.6539	16.9502
6	-0.9837	2.5829	17.9198
1	1.7500	4.4529	17.0204
1	-1.7432	2.5495	18.7265
6	0.0132	3.5790	17.9715
6	0.0875	4.5445	19.1255
8	0.9458	5.4397	19.1729
8	-0.8331	4.3095	20.0523
1	-0.7350	5.0108	20.8703
7	-0.6175	5.9841	21.9812
1	1.0355	6.6985	20.9501
1	-2.2847	5.3766	23.1092
6	0.3976	6.8719	21.8515
6	-1.4629	6.1224	23.0268
6	0.6043	7.9225	22.7560
6	-1.3494	7.1538	23.9667
1	1.4480	8.6275	22.6102
1	-2.0973	7.2460	24.7915
6	-0.2918	8.0832	23.8401
16	-0.1244	9.5343	24.8588
79	-0.0456	1.7633	27.0399
79	2.8013	1.7510	26.9823
79	5.7670	1.7400	26.9366
79	1.3992	4.2608	27.0874
79	4.2897	4.2868	27.1614
79	7.1711	4.2556	27.0713
79	2.8489	6.7421	27.0412
79	5.7239	6.7431	27.0904
79	8.6167	6.7307	27.1420
79	1.4365	0.9728	29.5457
79	4.3012	0.9660	29.5811
79	7.1645	0.9666	29.5391
79	2.8591	3.4489	29.6196
79	5.7404	3.4460	29.6074
79	8.6248	3.4522	29.6243
79	4.2985	5.9653	29.6550
79	7.1804	5.9523	29.6463
79	10.0728	5.9530	29.6393
79	-0.0197	0.1328	32.0715
79	2.8618	0.1223	32.1174

79	5.7488	0.1225	32.1080
79	1.4214	2.6122	32.1144
79	4.3054	2.6138	32.1264
79	7.1888	2.6130	32.1035
79	2.8615	5.1113	32.1338
79	5.7481	5.1114	32.1319
79	8.6317	5.1129	32.1310
79	-0.0148	1.7491	34.6287
79	2.8681	1.7509	34.6385
79	5.7555	1.7507	34.6305
79	1.4270	4.2484	34.6456
79	4.3117	4.2511	34.6434
79	7.1965	4.2477	34.6403
79	2.8726	6.7494	34.6244
79	5.7512	6.7484	34.6301
79	8.6386	6.7466	34.6393
79	1.4348	0.8787	37.1553
79	4.3194	0.8800	37.1532
79	7.2023	0.8788	37.1519
79	2.8770	3.3770	37.1579
79	5.7613	3.3766	37.1547
79	8.6442	3.3763	37.1578
79	4.3185	5.8758	37.1570
79	7.2020	5.8757	37.1575
79	10.0882	5.8764	37.1571

$(CHO_2)_2Ph_2$

CRYSTAL
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4.3260 7.4929 0.0000
0.0000 0.0000 39.0000
PRIMCOORD
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79	2.8840	0.0000	0.0000
79	5.7680	0.0000	0.0000
79	1.4420	2.4976	0.0000
79	4.3260	2.4976	0.0000
79	7.2100	2.4976	0.0000
79	2.8840	4.9952	0.0000
79	5.7680	4.9952	0.0000
79	8.6520	4.9952	0.0000
79	-0.0179	1.6545	2.5200
79	2.8667	1.6551	2.5267
79	5.7488	1.6540	2.5269
79	1.4261	4.1510	2.5224
79	4.3068	4.1516	2.5272
79	7.1917	4.1522	2.5147
79	2.8664	6.6501	2.5230
79	5.7499	6.6501	2.5197
79	8.6340	6.6523	2.5219
79	1.3902	0.8059	5.0364
79	4.2731	0.8108	5.0579
79	7.1566	0.8061	5.0403
79	2.8358	3.3001	5.0592
79	5.7142	3.3023	5.0465
79	8.5997	3.3035	5.0293

79	4.2738	5.7996	5.0405
79	7.1581	5.8007	5.0288
79	10.0423	5.8010	5.0355
79	-0.1135	-0.0592	7.5529
79	2.7708	-0.0577	7.5472
79	5.6591	-0.0537	7.5641
79	1.3298	2.4379	7.5485
79	4.2241	2.4453	7.6314
79	7.0967	2.4379	7.5599
79	2.7778	4.9371	7.5656
79	5.6541	4.9364	7.5597
79	8.5413	4.9375	7.5393
79	-0.1907	1.5637	10.0635
79	2.7054	1.5706	10.0544
79	5.5996	1.5562	10.1460
79	1.2598	4.0563	10.0287
79	4.1402	4.0850	10.1492
79	7.0220	4.0620	10.0469
79	2.7034	6.5645	10.0850
79	5.5770	6.5592	10.0618
79	8.4616	6.5684	10.0269
79	1.1875	0.6965	12.5461
79	4.0387	0.6828	12.6353
79	6.9045	0.7263	12.6797
79	2.6019	3.1726	12.6379
79	5.5060	3.1890	12.6616
79	8.3847	3.1922	12.6068
79	4.0742	5.6329	12.6852
79	6.9487	5.6800	12.5972
79	9.8010	5.6684	12.5093
16	-1.0516	-0.5927	14.7571
6	0.3560	0.2512	15.4579
1	1.6351	-1.5248	15.4263
1	-0.6928	2.1665	15.5894
6	1.5347	-0.4730	15.7726
6	0.2242	1.6037	15.8649
6	2.5368	0.1313	16.5400
6	1.2297	2.1982	16.6353
1	3.4566	-0.4171	16.8284
1	1.1368	3.2429	16.9955
6	2.3708	1.4535	17.0021
6	3.3584	2.0161	17.9654
8	4.3412	1.2963	18.3229
8	3.1103	3.2090	18.4109
1	3.8092	3.5108	19.2421
1	5.0791	1.7261	19.3157
8	5.7513	2.0094	20.1713
8	4.5386	3.9367	20.2379
6	5.4827	3.1891	20.6411
6	6.3937	3.6943	21.7054
1	7.6146	1.8951	21.7161
1	5.2959	5.5571	21.9048
6	7.4945	2.9182	22.1260
6	6.1885	4.9859	22.2343
6	8.4306	3.4582	23.0145
6	7.1201	5.5353	23.1217
1	9.3189	2.8744	23.3376
1	6.9917	6.5619	23.5273
6	8.2715	4.7885	23.4784
16	9.6409	5.5932	24.2863
79	0.1265	1.7527	26.3914
79	3.0054	1.7554	26.3577

79	5.9089	1.7715	26.3773
79	1.6036	4.2160	26.3479
79	4.4728	4.2605	26.3748
79	7.3240	4.2468	26.4470
79	3.0414	6.7704	26.5121
79	5.8898	6.7559	26.3991
79	8.7605	6.8030	26.3504
79	1.5167	0.8938	28.9540
79	4.3989	0.8748	28.8758
79	7.2805	0.9021	28.9800
79	2.9420	3.3988	28.8758
79	5.8361	3.3876	28.9527
79	8.7308	3.3944	28.9371
79	4.4058	5.8807	28.9804
79	7.2899	5.8903	28.9387
79	10.1653	5.8864	28.9383
79	0.0426	0.0419	31.4611
79	2.9289	0.0427	31.4428
79	5.8058	0.0422	31.4522
79	1.4862	2.5414	31.4423
79	4.3597	2.5343	31.3885
79	7.2542	2.5415	31.4527
79	2.9247	5.0330	31.4522
79	5.8132	5.0378	31.4534
79	8.6963	5.0381	31.4530
79	0.0216	1.6906	33.9696
79	2.9070	1.6922	33.9562
79	5.7866	1.6944	33.9507
79	1.4636	4.1880	33.9652
79	4.3486	4.1848	33.9506
79	7.2304	4.1881	33.9636
79	2.9060	6.6867	33.9729
79	5.7891	6.6868	33.9701
79	8.6725	6.6873	33.9657
79	1.4507	0.8422	36.4832
79	4.3348	0.8423	36.4753
79	7.2163	0.8431	36.4812
79	2.8928	3.3398	36.4749
79	5.7754	3.3389	36.4769
79	8.6596	3.3394	36.4800
79	4.3342	5.8347	36.4810
79	7.2177	5.8368	36.4802
79	10.1010	5.8365	36.4806

S2. Details of the procedure to parameterize the anharmonic self-energy

We summarize the step-by-step procedure to evaluate the color noise term $\tau_a^{-1}(\omega, T)$ given in Section II.

(1) Calculate the phonon energy and normal mode vectors defined on the molecular junction's unit cell (i.e., Bloch state of phonon) using the frozen phonon approximation.

(2) Set the initial condition of each sampling based on the law of equipartition of energy, where the temperature is set to *T*. Each normal mode in a sampling state receives energy randomly distributed between kinetic energy (momentum in the normal model) and harmonic potential energy (amplitude in the normal mode).

(3) Transform the coordinates and velocities of the normal modes to real space for all normal modes defined over the supercell. This supercell must be the same as the cell used for the force constant matrix in the frozen phonon calculation.

(4) Carry out NVE-MD of the sampling states in real space and evaluate the relaxation time constants of all normal modes.

Since the initial parameter τ_{0a} is defined for each atomic species, not normal mode, we need to identify the normal modes dominated by the atomic species *a* and consider the averaged value of the vibrational relaxation times. Thus, the next step is:

(5) Select the normal modes to evaluate the parameter of atomic species *a* based on the following criteria:

$$c_1 < \frac{\sum_{\mu \notin I_{\mathrm{Au}}} \left(q_\mu^Q\right)^2}{\sum_\mu \left(q_\mu^Q\right)^2}\ ,\ c_2 < \frac{\sum_{\mu \notin I_{\mathrm{a}}} \left(q_\mu^Q\right)^2}{\sum_{\mu \notin I_{\mathrm{Au}}} \left(q_\mu^Q\right)^2}, \qquad \text{(S1)}$$

where Q is the label of the examined normal mode and q_μ^Q is the component of its normal mode vector. The criteria values (c_1, c_2) are (0.2,0.4) for C and H atoms, while (c_1, c_2) are taken as (0.05, 0.1) for O, N, and S atoms, respectively.

Here, we did not refer to the normal modes with frequencies higher than 36.0 THz since such high-frequency modes are not coupled with the electrodes and are not crucial for thermal transport. Typically, the frequencies of the normal modes that satisfy the criteria Eq. (S1) are lower than 10.0 Hz.

(6) Evaluate the relaxation time constant of the selected normal modes. Then set the initial $\tau_{0\alpha}^{-1}$ by averaging over the selected normal modes. One can use the following weight to average the values of each selected mode, Q_α.

$$w_{Q_\alpha} = \frac{\sum_{\mu \in I_a} (q_\mu^{Q=Q_\alpha})^2}{\sum_Q \sum_{\mu \in I_a} (q_\mu^Q)^2} \qquad \text{(S2)}$$

(7) Evaluate the set of approximated random forces $\xi_\mu(t)$ by the MD results as follows:

$$\xi_\mu(t) \sim F_\mu + \frac{1}{2} \sum_{\boldsymbol{\nu}} K_{\boldsymbol{\mu\nu}}\, x_\nu + M_\mu \Gamma_{0\alpha} \frac{dx_\mu}{dt}. \qquad \text{(S3)}$$

F_μ is the force acting on each DoF during the MD calculation like position and velocity. The colored noise and the resulting $\tau_\alpha^{-1}(\omega, T)$ are determined as a function of ω and T via the fluctuation-dissipation theorem.

Note that we used the value of $\tau_{0\alpha}^{-1} (= \Gamma_{0\alpha})$ obtained in step (6), where the temperature was set to 400 K, as the temperature-independent constant. Thus, the next cycle of calculations to determine the color noise at different temperatures requires only steps (2), (3), (4), and (7).

Here, we performed first principles MD in the above protocol, where SIESTA program package was used. Adopted basis set and XC functionals are same with those used for atomic structure optimization given in S1. MD trajectories were run typically for 20 ps, which is much shorter than time scale require for thermal transport calculation. The time step was set to 2.0 fs.

S3. The calculated plot of $\tau_a^{-1}(\omega,T)$ and their model functions

As stated in Sections II and III, the calculated $\tau_a^{-1}(\omega,T)$ is expressed by the model function:

$$\tau_a^{-1}(\omega,T)\sim\Gamma_{0a}f_a(\omega,T)$$

$$f_a(\omega,T) = A\sinh(\alpha_T T) + B\tanh(\beta_T T)\sinh(\alpha_\omega \omega) \qquad \text{(S4)}$$

Here, we found that the transmission coefficient by ballistic approximation is almost zero when the energy (frequency) is higher than 7.0 THz. This is consistent with the phonon DOS of Au bulk or (111) zero above 5.0 THz. Thus, we used data only in the range $0 < \omega < 7.0$ Hz to determine the model parameters. The resulting color noise of the atomic species C, i.e., the term $\tau_{a=\mathrm{C}}^{-1}(\omega,T)/\Gamma_{0a}$ and the related model function $f_{a=\mathrm{C}}(\omega,T)$, are plotted in Figure S3-1.

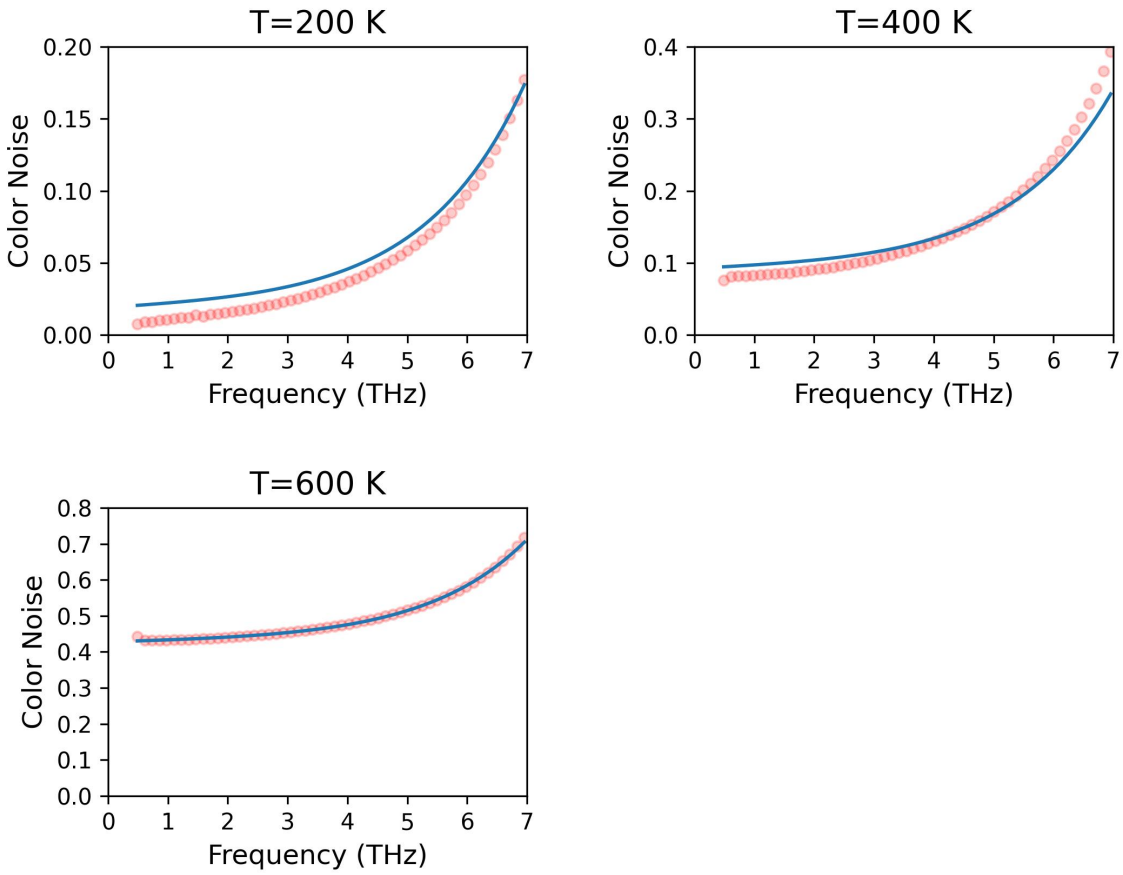

Figure S3-1. Plots of the color noise related to anharmonicity for atomic species C. All plots are a function of frequency, with the temperature set to 200 K (top left), 400 K (top right), and 600 K (bottom left). The thin red circles represent the calculated results from MD data, and the blue lines represent the plots by the model function.

S4. Phonon DOS and transmission coefficient of elastic term with and without anharmonic effect

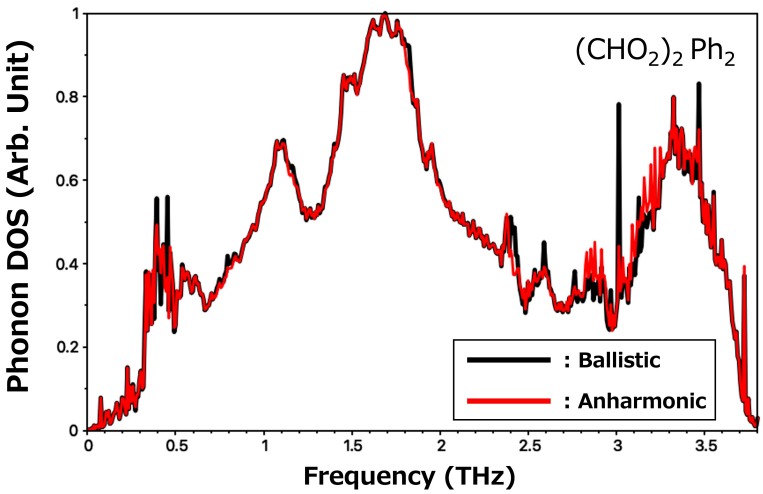

Figure S4-1. Plots of the phonon DOS of $(CHO_2)_2Ph_2$ junction. The black line is the result of ballistic approximation, i.e., DOS without anharmonic effect. The red line represents DOS including anharmonic effect where temperature is set to 500 K.

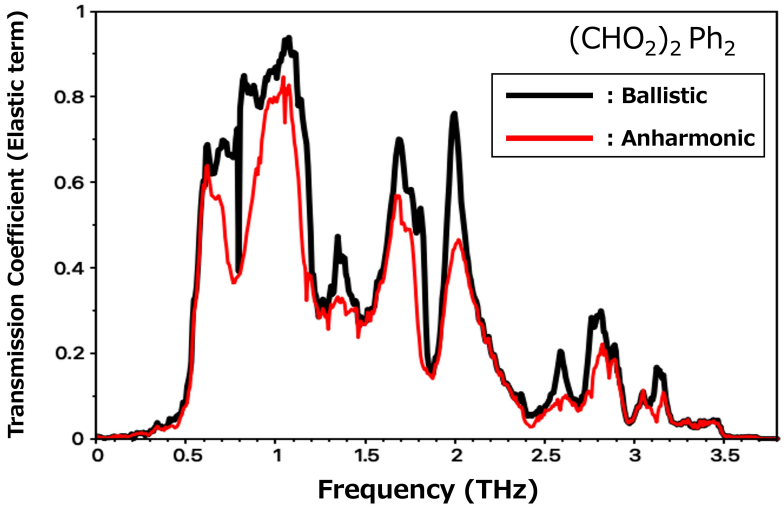

Figure S4-2. Plots of the transmission coefficient of elastic term in Eq. (4), $\mathcal{T}^{ela}$, of $(CHO_2)_2Ph_2$ junction. The black and red lines are the result of ballistic approximation and that with anharmonic effect of 500K, respectively.

S5. Electric conductance and electric thermal conductance

Thermal conductance by electric transport of a molecular junction is evaluated as

$$\kappa_e = \frac{1}{2\pi T}\left(L^{(2)} - \frac{(L^{(1)})^2}{L^{(0)}}\right) \qquad \text{(S5)}$$

where e and $\hbar$ are set to 1. The coefficient $L^{(n)}$ can be calculated by integral of electron energy E,

$$L^{(n)} = \frac{1}{2\pi}\int dE \left(-\frac{\partial f_{FD}(E,T)}{\partial E}\right)(E - E_F)^n \mathrm{T}_e(E) \qquad \text{(S6)}$$

$f_{FD}(E,T)$ is Fermi-Dirac function and E_F is Fermi level of the system.[2] $\mathrm{T}_e(E)$ is the transmission coefficient of *electron*. The transmission coefficient can be calculated NEGF combined with DFT (NEGF-DFT), where Green's function is electric Green's function by DFT instead of phonon Green's function. Details of NEGF-DFT is given in Refs. We performed NEGF-DFT for $(CHO_2)_2Ph_2$ junction. In Figure S5, the plot of calculated $\mathrm{T}_e(E)$ is shown around E_F. Using calculated $\mathrm{T}_e(E)$ and Eqs (S5) and (S6), we found that $\kappa_e(T = 300K)$ was 1.72×10^{-1} pW/K.

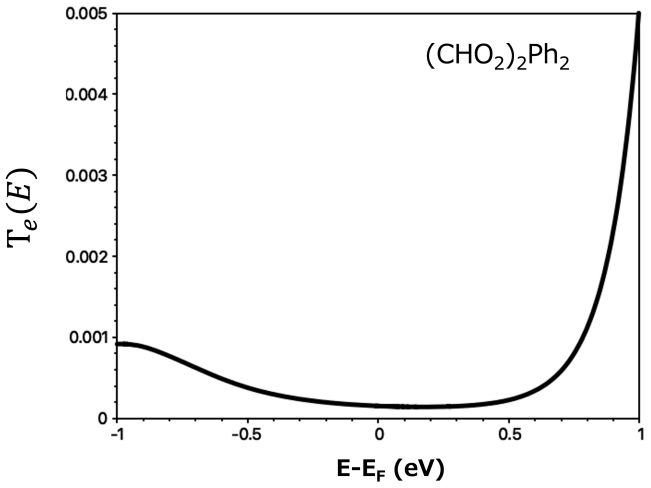

Figure S5. Plots of the transmission coefficient of electric transmission coefficient of $(CHO_2)_2Ph_2$ junction calculated by NEGF-DFT with ballistic approximation.

S6. Transmission coefficient of elastic term of forward and backward direction

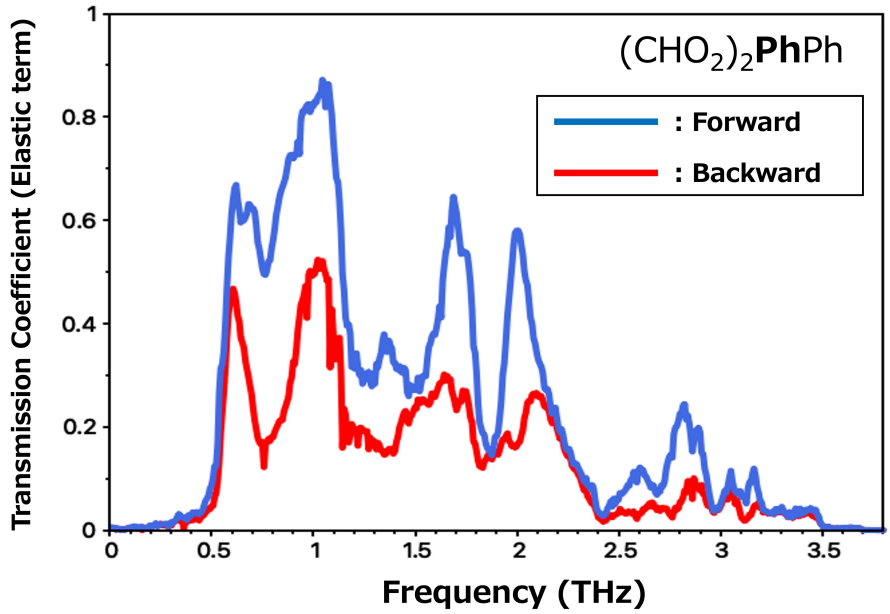

Figure S6. Plots of the transmission coefficient of elastic term, $\mathcal{T}^{ela}$, of $(CHO_2)_2$**Ph**Ph junction. The blue line is the result of positive temperature bias, i.e., D^H side is connected low temperature electrode. The red line represents $\mathcal{T}^{ela}$ for negative temperature bias, i.e., D^H side is in high temperature regime and reduction of the transmission coefficient is enhanced by dephasing effect of anharminicity.

References

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(2) Bergfield, J. P.; Stafford, C. A. Thermoelectric signatures of coherent transport in single-molecule heterojunctions. *Nano Lett* **2009**, *9* (8), 3072-3076. DOI: 10.1021/nl901554s From NLM PubMed-not-MEDLINE.