Electronic Supplementary Information

Dependence of Electron Transfer Dynamics on the Number of Graphene Layers in π-stacked 2D Materials: Insights from Ab Initio Nonadiabatic Molecular Dynamics

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S1. Electronic structure convergence study.

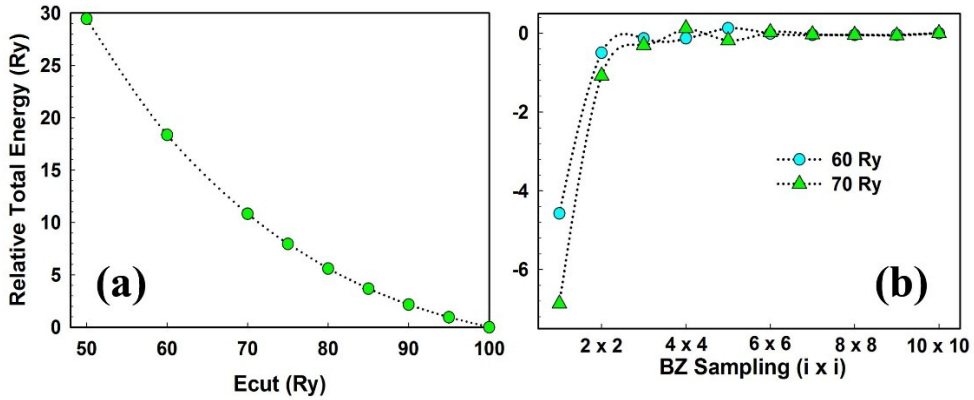

Figure S1. Total energies relative to final points as functions of cut-off energy (a) and Monkosrt-Pack grid of Brillouin zone (b). Here, the U_d=7.0 eV is used for Zn atom and U_p = 5.5 eV is used for both C and N atoms.

S2. Justification of the NBRA method.

To assess the validity of the NBRA approach, we have optimized the ZnPc/SLG system on the ground and first and second electronic states. Because of the system's complexity, we could afford only a simple ΔSCF approach. As our starting excited state corresponds to the neutral exciton on ZnPc via H-2 → L+2 excitation, the ΔSCF calculations are performed by removing one electron from the system's H-2 orbital and placing it to L+2 orbital. For the second excited state, one electron is removed from the system's H-2 orbital and placed to L+3 orbital. The 3x3x1 k-point grid and 60 Ry kinetic energy cutoff are utilized. Hubbard +U correction is used, with values of U = 7.0 eV for Zn and U = 5.5 eV for both C and N, and Grimme's dispersion correction added to PBE functional.

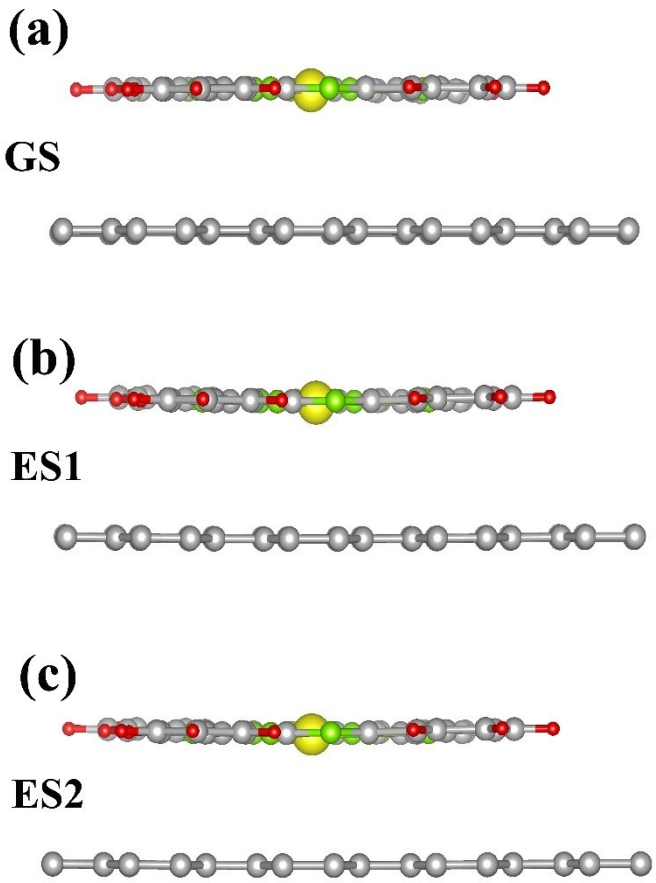

Figure S2. Optimized geometries of ground (a), first excitation (b), and second excited states. Here, the energy cutoff is 60 Ry, and a 3x3x1 Monkhorst-Pack mesh is used. Also, the U_d=7.0 eV is used for Zn atom and U_p = 5.5 eV is used for both C and N atoms.

The resulting structures are shown in Fig. S2. No significant distortions are observed in this system. This means the excited and ground state forces are comparable and maybe nearly parallel to each other, which is a good basis for NBRA. The computed energies are given in Table S1 below.

Table S1. Energetics of ZnPc/SLG on the ground and excited states. Here, $^{E_{gs}}$ and $^{E_{ex}}$ refer to energies of the ground and excited states, respectively, $^{R_{gs}}$ and $^{R_{ex}}$ refer to the energy minimum geometries for the ground and excited states, respectively. The reorganization energy is computed as $\lambda = E_{ex}(R_{gs}) - E_{ex}(R_{ex})$, and the vertical excitation energy is computed as $\Delta E = E_{ex}(R_{gs}) - E_{gs}(R_{gs})$. The calculated $^{E_{gs}(R_{gs})}$ is -1712.9626 Ry.

	$E_{ex}(R_{gs})$, Ry	$E_{ex}(R_{ex})$, Ry	λ, eV	ΔE, eV
Energy (ES1)	-1712.8246	-1712.8340	0.128	1.88
Energy (ES2)	-1712.8162	-1712.8296	0.182	1.99

S3. Determining the uncertainty in computed timescales.

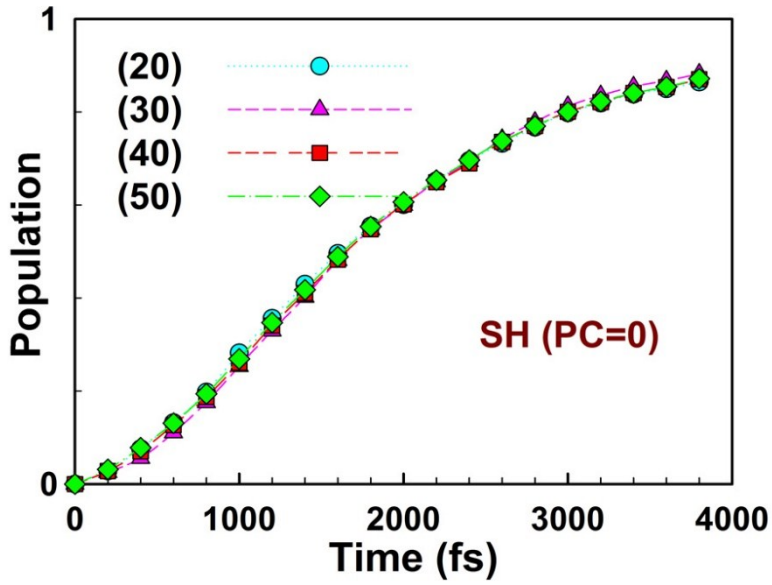

Figure S3. Time evolution of total population of CT-type configurations computed with FSSH method using different numbers of initial configurations. Circle, triangle, square, and diamond are for 20, 30, 40, and 50 numbers of initial conditions randomly selected for averaging the population over the canonical ensemble.

S4. Resolving the distortion of interface.

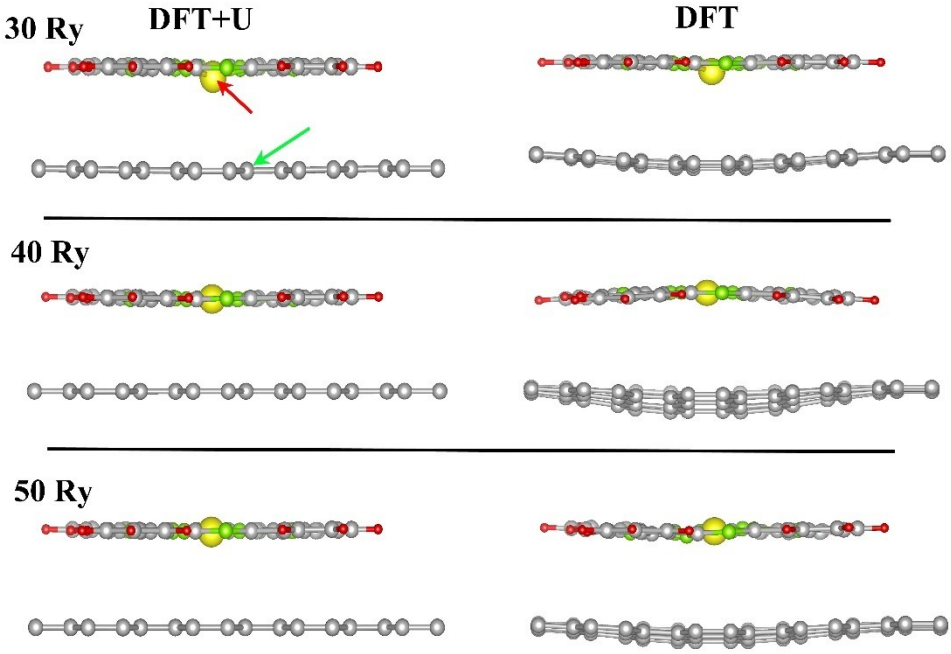

Figure S4. Relaxed geometries of ZnPc/SLG interface using three cutoff energies of 30, 40, and 50 Ry (first, second and third rows, respectively) with DFT+U and pure DFT. The arrows show the slight distortions in the planar structures of ZnPc and SLG relaxed at DFT+U level of theory. Here, a 3x3x1 Monkhorst-Pack mesh is used. Also, the U_d=7.0 eV is used for Zn atom and U_p = 5.5 eV is used for both C and N atoms.

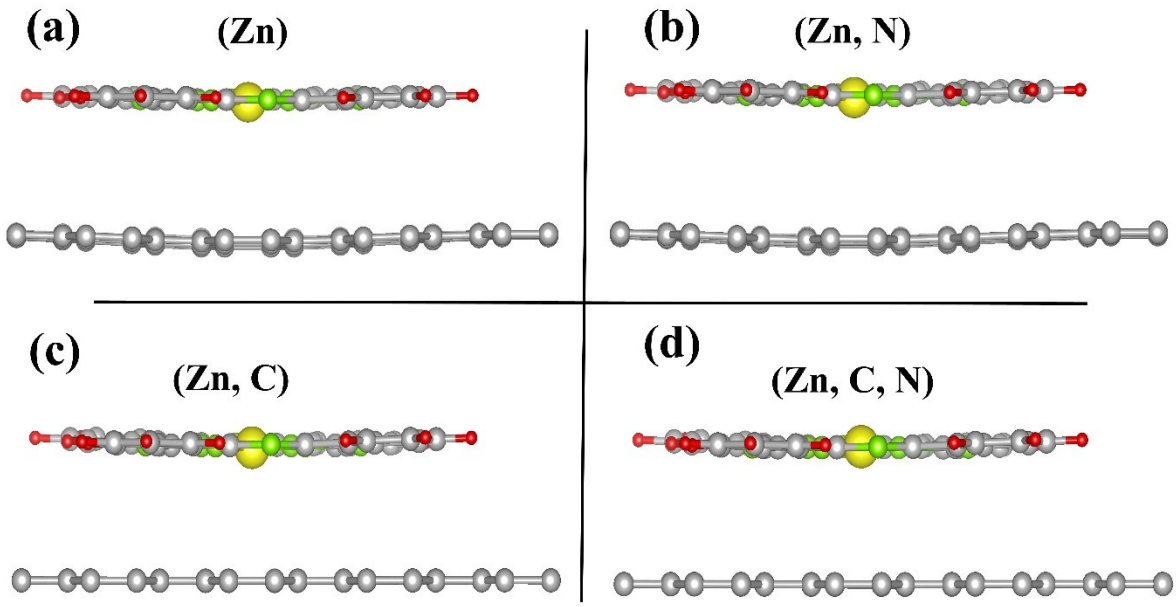

Figure S5. Relaxed geometries of ZnPc/SLG interface using DFT+U model with U terms used for: (a) Zn; (b) Zn and N; (c) Zn and C atoms; (d) and Zn, C, and N atoms. Here, the energy cutoff is 60 Ry, and Monkhorst-pack mesh of 3x3x1 is used. Also, the U_d=7.0 eV is used for Zn atom and U_p = 5.5 eV is used for both C and N atoms.

S5. Tracking the orbitals' identities.

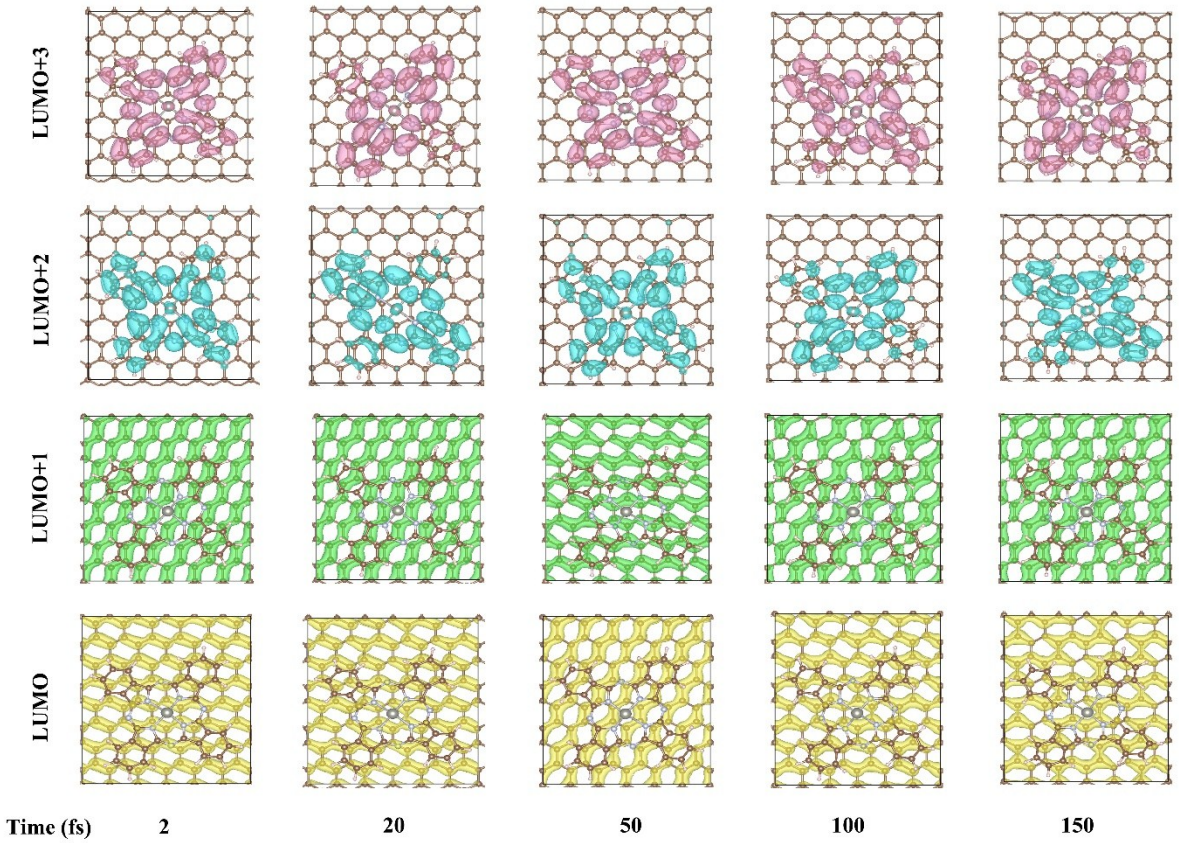

Figure S6. Snapshots of the charge density distributions of frontier unoccupied orbitals for ZnPc/SLG system at $T = 300\ K$ taken at representative time steps of MD trajectory. The kinetic energy cut-off of 80 Ry and Brillioun zone was sampling with the $8 \times 8 \times 1$ Monkhorst-Pack mesh are used. Also, the U_d=7.0 eV is used for Zn atom and U_p = 5.5 eV is used for both C and N atoms. One can observe trivial crossings of nearly-degenerate donor orbitals (LUMO+2 and LUMO+3) among each other (e.g. 100 fs to 150 fs), as well as trivial crossings of nearly-degenerate acceptor levels (LUMO and LUMO+1, e.g. 20 fs to 50 fs snapshot).

S6. Electronic structure calculations on the ZnPc/DLG system.

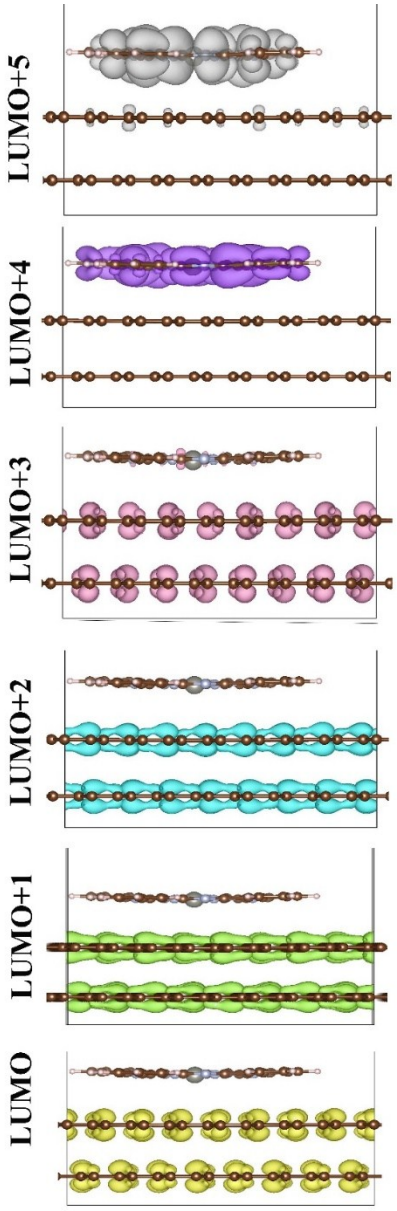

Figure S7. Charge density distributions of frontier unoccupied orbitals for ZnPc/DLG system at $T = 0\,K$. The kinetic energy cut-off of 80 Ry and Brillouin zone sampling with the $8 \times 8 \times 1$ Monkhorst-Pack mesh are used. Also, the U_d=7.0 eV is used for Zn atom and U_p = 5.5 eV is used for both C and N atoms.

S7. Energy levels shifts and NAC rescaling

The KS energy levels have been shifted using the scissor operator, as implemented in the Libra/NBRA module. An example of input for SLG system is:

shifting the energy levels
data_conv.scissor(Hvib, 0, -1.07/27.2114) # all SD state energies are lowered by -1.06 eV as a result of lowering energy of ZnPc's H state by -1.06 eV

data_conv.scissor(Hvib, 2, -0.33/27.2114) # energies of 2 and 3 SD states are lowered more by -0.33 eV as a result of lowering energies of ZnPc's L and L+1 states by -0.33 eV

Following the energy levels' shifts, the NACs have been rescaled based on the changes in the gaps between the levels, as suggested by Lin and Akimov:[1]

$$NAC_{after} = NAC_{before}\frac{E_{ij,before}}{E_{ij,after}}.$$

An example of input for DLG system is:

…..
Hvib = step3.run(S, St, Hvib_ks, params)
# rescaling the SD NACs
data_conv.scale_NAC(Hvib, 0, 2, 0.66/0.33) # - rescale NAC between Phi_0 and Phi_2
data_conv.scale_NAC(Hvib, 2, 0, 0.66/0.33) # - rescale NAC between Phi_0 and Phi_2
data_conv.scale_NAC(Hvib, 0, 3, 0.75/0.42) # - rescale NAC between Phi_0 and Phi_3
data_conv.scale_NAC(Hvib, 3, 0, 0.75/0.42) # - rescale NAC between Phi_0 and Phi_3
data_conv.scale_NAC(Hvib, 1, 2, 0.56/0.23) # - rescale NAC between Phi_1 and Phi_2
data_conv.scale_NAC(Hvib, 2, 1, 0.56/0.23) # - rescale NAC between Phi_1 and Phi_2
data_conv.scale_NAC(Hvib, 1, 3, 0.65/0.32) # - rescale NAC between Phi_1 and Phi_3
data_conv.scale_NAC(Hvib, 3, 1, 0.65/0.32) # - rescale NAC between Phi_1 and Phi_3

The cumulative effect of energy shifts is represented in Figure S5.

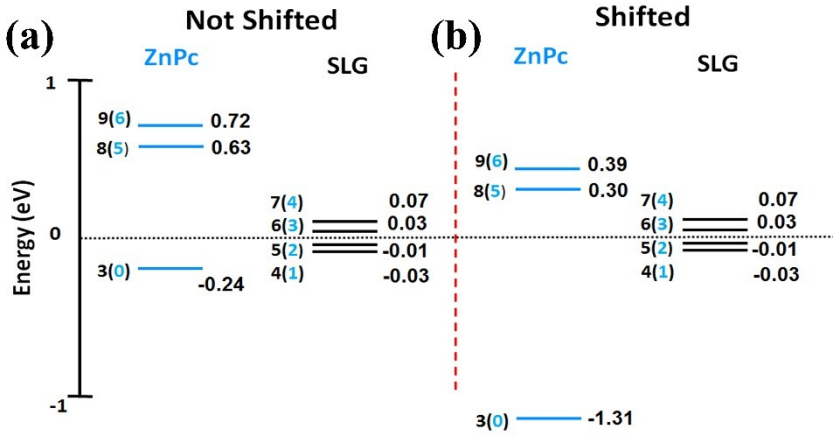

Figure S8. The energy level diagrams for KS orbitals included in the active space for (a) ZnPc/SLG and (b) ZnPc/DLG systems. The left side of each panel shows the energy levels before shifts, the right side – after the shifts. The energies are obtained by averaging over the 4 ps long NVE trajectory. The kinetic energy cut-off of 60 Ry and Brillouin zone sampling at gamma are used. Also, the U_d=7.0 eV is used for Zn atom and U_p = 5.5 eV is used for both C and N atoms.

Energy shifts and NAC rescaling are applied for all configurations along the computed MD trajectory. The time-dependent orbital energy levels before and after shifts are shown in Figure S6.

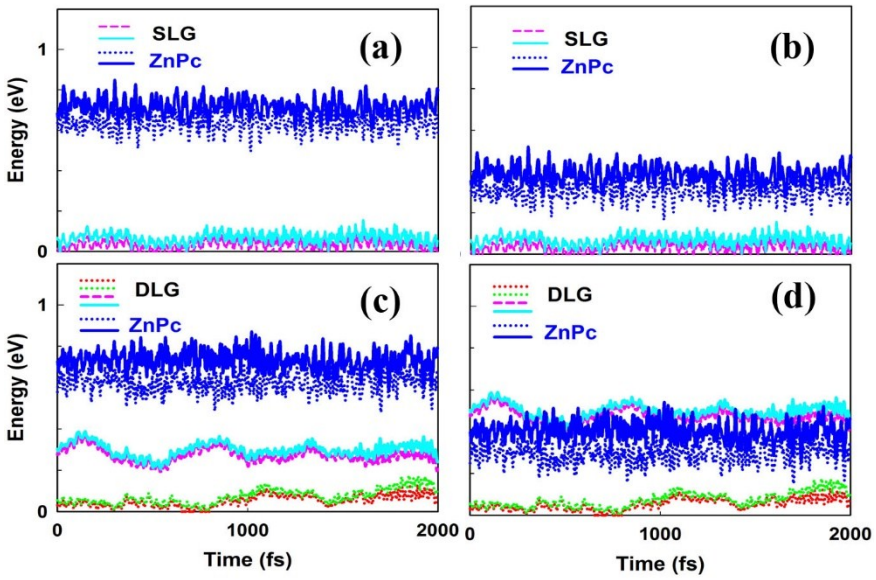

Figure S9. Time evolutions of unshifted and shifted electronic levels in the total conduction manifold of ZnPc/SLG ((a) and (b)) and ZnPc/DLG ((c) and (d)) interfaces. Shifted electronic levels of ZnPc and DLG are displayed in the right panels. The time evolution is first half of the 4 ps NVE trajectory. The kinetic energy cut-off of 60 Ry and Brillouin zone sampling at gamma are used. Also, the U_d=7.0 eV is used for Zn atom and U_p = 5.5 eV is used for both C and N atoms.

The large observed band downshift magnitude is likely a reflection of the limitations of the KS-DFT method for describing excited states of the studies systems. It is likely that a multi-configurational treatment of ZnPc's excited states, as well as the accounting for multiple k-points in graphene layers, may be needed for more accurate modeling of this challenging system, but such capabilities are out of computational feasibility at the moment.

S8. The reproducibility tests

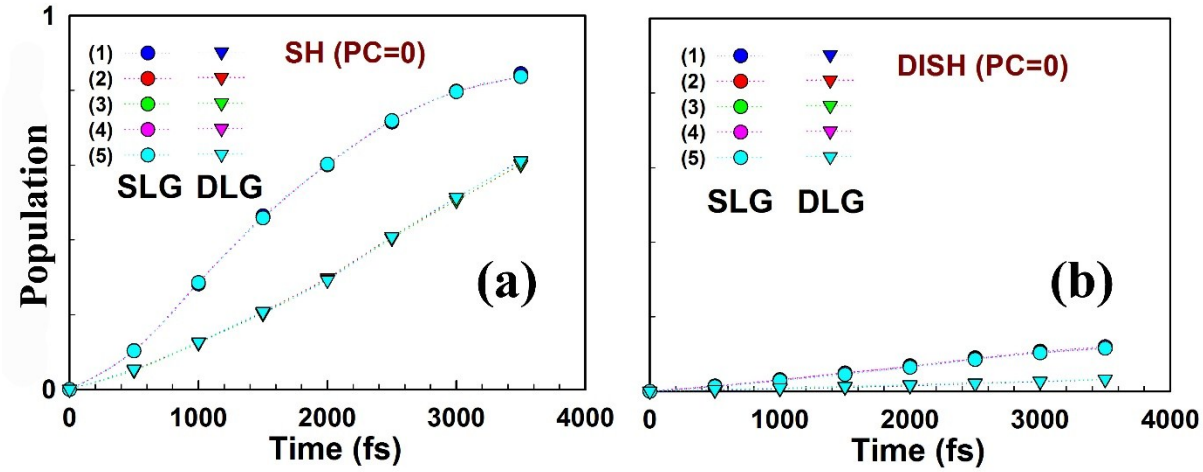

Figure S10. The NAMD dynamics of electron injection from the ZnPc molecule to FLG. The NAMD calculations are repeated five times using FSSH and DISH models for both ZnPc/SLG (circle) and ZnPc/DLG (triangle) interfaces. PC=0 denotes ET dynamics without phase correction of the adiabatic states.

S9. The effect of phase correction on NACs

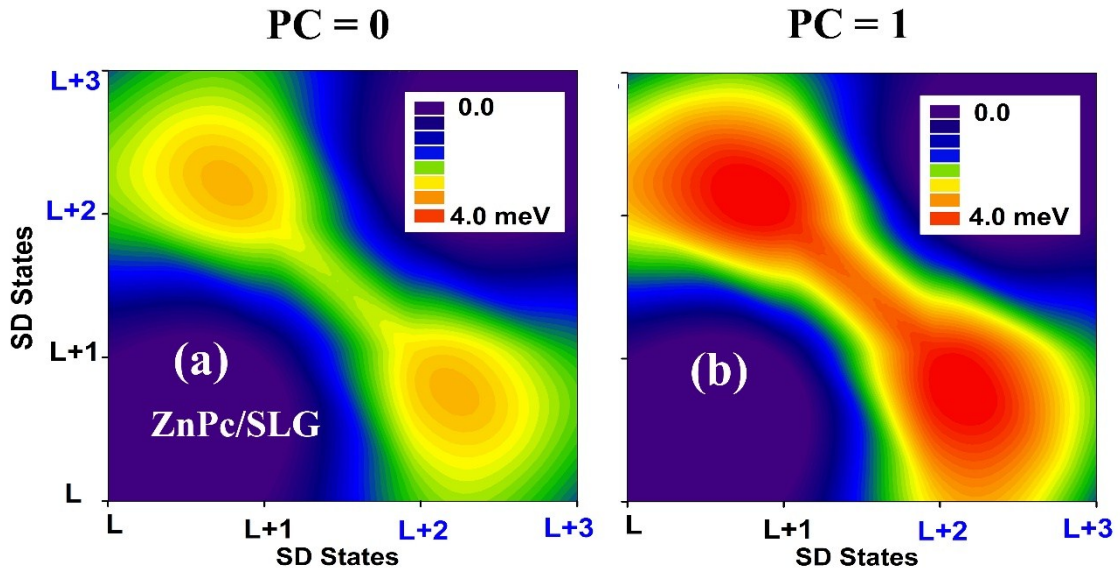

Figure S11. Contour plot of non-diabatic coupling (NAC) between electronic multi-electron states contributing in ET at the ZnPc/SLG interface. The black and blue colored indexes denote ES and TS states (initial excitation in ZnPc and transferred electron states in SLG), respectively. The very large NACs between SD states related to transition within ZnPc or SLG have been set to zero.

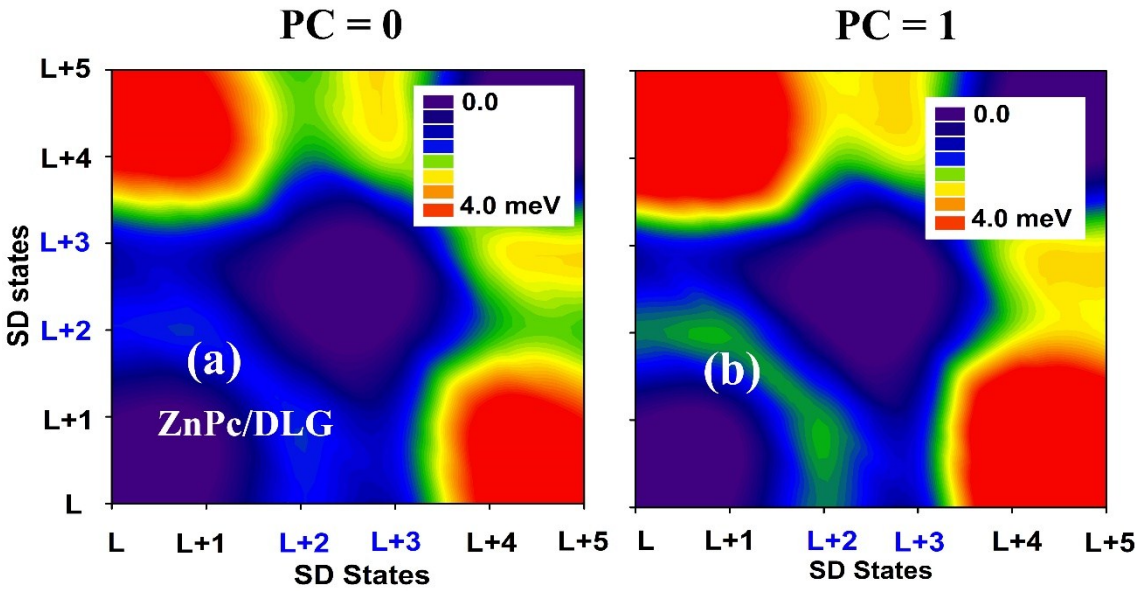

Figure S12. Contour plot of non-diabatic coupling (NAC) between electronic multi-electron states contributing in ET at the ZnPc/DLG interface. The black and blue colored indexes denote ES and TS states (initial excitation in ZnPc and transferred electron states in DLG), respectively. The very large NACs between SD states related to transition within ZnPc or DLG have been set to zero.

S10. The role of the energy levels alignment.

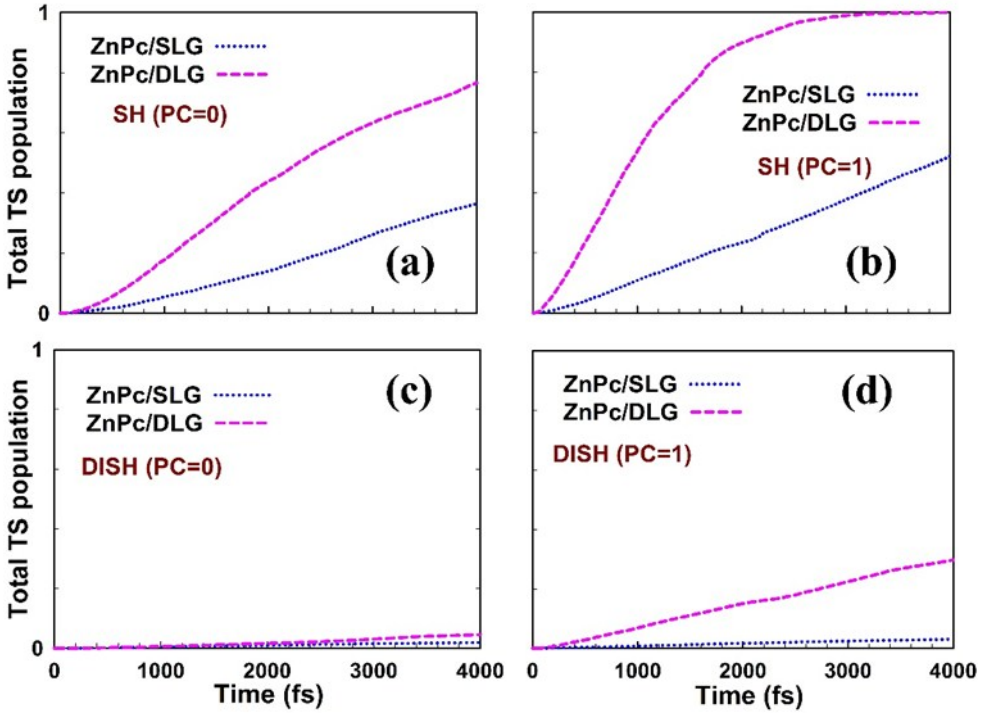

Figure S13. The dynamics of electron injection from the ZnPc molecule to FLG obtained using SH and DISH models and accounting for phase correction when the energy level shift is not applied: the curves show the total population of the ET states in ZnPc/SLG (solid curves) and ZnPc/DLG (dotted curves) interfaces. PC =0 and 1 denote ET dynamics without and with the implementation of the phase correction of the adiabatic states.

S11. Optimized ZnPc/SLG and ZnPc/DLG supercells.

Table S2. Optimized Cartesian atomic positions of the ZnPc/SLG hybrid. Orthorhombic, $a = 14.76$ Å, $b = 17.04$ Å, $c = 20.00$ Å, (153 atoms).

Atom	x	y	z
C	0.000823956	-0.012695247	2.074137767
C	0.000725856	1.407096109	2.053040397
C	2.461336257	-0.012334942	2.059842106
C	2.461835957	1.407095877	2.038059984
C	1.231393399	2.117123878	2.034981521
C	1.231197573	3.536690292	2.006369090
C	0.000473090	4.246418915	1.996553921
C	0.000608264	5.666450217	1.981511353
C	4.920977641	-0.012177231	2.026772236
C	4.921120387	1.406871927	2.007965617
C	3.691509894	2.117001344	2.010819103
C	3.691385833	3.536276754	1.990811048
C	2.461693915	4.246370510	1.989441039
C	2.461463158	5.666118363	1.976989161
C	1.231154026	6.376672531	1.976666411
C	1.231359932	7.796101634	1.975886048
C	0.000994807	8.506804634	1.981270366
C	0.001183359	9.926377665	1.995998110
C	7.380795663	-0.012766878	2.011398035
C	7.380715149	1.406991794	1.997884531
C	6.150903659	2.117028956	1.991211587
C	6.151146538	3.536406449	1.978027370

Table S2. continued from previous page

C	4.921058823	4.246421120	1.977597825
C	4.920596245	5.666104403	1.968850639
C	3.690897279	6.376551693	1.969855404
C	3.690664409	7.795953339	1.968687609
C	2.461253624	8.506988866	1.974543948
C	2.461170911	9.926027851	1.987115806
C	1.231383140	10.636350114	2.004174670
C	1.231255614	12.055594231	2.033582453
C	0.000979720	12.765660030	2.052033416
C	0.000852988	14.185881389	2.073611182
C	9.840815770	-0.012773329	2.028068300
C	9.840972660	1.406834645	2.011715852
C	8.610789409	2.117319230	1.994151487
C	8.610992607	3.536514509	1.978128338
C	7.381070569	4.246247797	1.970449375
C	7.381005294	5.666170609	5.666170609
C	6.150685712	6.376610726	1.961902031
C	6.150441908	7.796017971	1.961147598
C	4.920374982	8.506815540	1.966967201
C	4.920419914	9.925910345	1.976433203
C	3.690621842	10.636245527	1.990055640
C	3.690754491	12.055700300	2.011783517
C	2.461362202	12.765729384	2.037958742
C	2.461216155	14.185732167	14.185732167
C	1.231097160	14.896636515	2.075875748
C	1.231147900	16.316488379	2.075912300

Table S2. continued from previous page

C	12.300463177	-0.012693981	2.060568939
C	12.300315661	1.407001041	2.039616118
C	11.070838555	2.117162229	2.012872243
C	11.070947368	3.536671018	1.990439955
C	9.841107417	4.246510835	1.976053827
C	9.841183341	5.666069984	1.966694052
C	8.611119731	6.376412410	1.961223803
C	8.610904486	7.795773711	7.795773711
C	7.380591490	8.506601520	1.962832146
C	7.380507807	9.926031706	1.971127265
C	6.150605935	10.636115574	1.978577511
C	6.150818773	12.055242652	1.994527726
C	4.920634349	12.765596184	2.011441904
C	4.920860937	14.185610998	2.027973862
C	3.691135963	14.896642707	2.050059750
C	3.691232069	16.316621420	2.050080638
C	13.530422929	2.117435372	2.035227622
C	13.530226466	3.536792639	2.005269980
C	12.300393870	4.246713638	1.987601539
C	12.300382911	5.666174642	1.974350801
C	11.070876705	6.376673400	1.968514779
C	11.070705764	7.795981703	1.969927965
C	9.840964828	8.506727725	1.969238929
C	9.840549618	9.925917384	1.978128982
C	8.610486745	10.636155632	1.978764299
C	8.610717452	12.055558594	1.991600121

Table S2. continued from previous page

C	7.380922240	12.765313844	1.998286621
C	14.185453072	14.185453072	2.011583560
C	6.150939005	14.896453941	2.020146325
C	6.150850244	16.316231737	2.019901297
C	13.530259698	6.376683853	1.975667450
C	13.530485008	7.796107470	7.796107470
C	12.300100169	8.506956539	1.976837417
C	12.299932740	9.926228382	1.989213227
C	11.070213379	10.636486689	1.990809897
C	11.070134018	12.055723703	2.010783580
C	9.840506635	12.765515871	2.008069333
C	9.840739110	14.185027742	2.026629338
C	8.610861568	14.896155274	2.019866510
C	8.610761663	16.315911290	2.020082721
C	13.530412793	10.636296319	2.005859450
C	13.530276419	12.055854956	12.055854956
C	12.299832912	12.765548690	12.765548690
C	12.300350746	14.185343510	2.059621663
C	11.070432692	14.895950155	2.049925547
C	11.070577138	16.315929055	2.050196313
C	13.530534475	14.896280261	2.075801323
C	13.530605857	16.316132043	2.076247753
Zn	7.350282943	7.107725005	5.389547882
N	5.757699178	8.299608585	5.415212370
N	6.825955906	10.411394407	5.427252057
N	4.111827124	6.597910789	5.430390449

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N	8.514900480	8.743934813	5.416311965
N	10.639159226	7.690927330	5.429542851
N	6.231247537	5.530711995	5.416837042
N	7.930971997	3.873482896	5.427078046
N	8.995913145	5.985454591	5.414909526
C	5.770600886	9.644243365	5.421923317
C	4.492175712	7.846764676	5.423166587
C	4.417633975	10.103139802	5.433520323
C	3.616140475	8.973914742	5.433924715
C	3.869959605	11.350119909	5.451493726
C	2.259614280	9.081052636	5.453235188
C	8.069014864	10.015249331	5.429735451
C	4.882696983	5.545735294	5.434198799
C	10.324907586	10.090145265	5.460258394
C	9.197701499	10.889727730	5.455698203
C	9.862355486	8.737375830	5.433062832
C	11.570864768	10.642130076	10.642130076
C	9.302265556	12.247890377	5.474922934
C	5.552564089	3.390607052	5.455939923
C	4.425246470	4.193877148	4.193877148
C	6.684341870	4.260182351	5.430034273
C	5.440058381	2.033395276	5.473622585
C	3.178259969	3.645950602	5.488937153
C	10.258124332	6.443683547	5.422374281
C	10.347728570	4.189808320	5.432934880
C	11.140716585	5.324900884	5.433110942

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C	8.988910902	4.639343571	5.421504575
C	10.918853976	2.952985928	5.451147373
C	12.499072551	5.240264892	5.452768575
C	1.717537264	10.332229035	5.467971918
C	2.510153118	11.450654146	5.466899057
C	4.189710064	1.493015476	5.497460978
C	3.072295654	2.287579793	5.505469856
C	13.060902601	3.999587802	5.469028560
C	12.280207717	2.872844750	5.467718848
C	10.550947195	12.793614310	5.499371518
C	11.669736924	12.002412900	5.505839343
H	2.303374632	4.290605240	5.494927099
H	6.331876032	1.410944720	5.466177922
H	10.297529795	2.060872077	5.455379489
H	13.102762109	6.145125137	5.458797153
H	12.452461702	10.006082334	5.493373213
H	8.406716572	12.864847419	5.468504402
H	4.511588328	12.228245599	5.456273840
H	1.640104030	8.187441466	5.459432887
H	2.090741174	1.819371230	5.521182308
H	4.070393648	0.412924326	5.505024162
H	12.760265590	1.898634757	5.482013380
H	14.142041630	3.894591520	5.485030971
H	12.648714013	12.473589837	5.522285584
H	10.667181005	13.874655155	5.508929874
H	2.040090769	12.431371826	5.480287064
H	0.637866463	10.452378086	5.482606487

H	2.760265590	1.898634757	5.482013380

Table S3. Optimized Cartesian atomic positions of the ZnPc/DLG hybrid. Orthorhombic, $a = 14.76$ Å, $b = 17.04$ Å, $c = 23.00$ Å, (249 atoms).

Atom	X	y	z
C	-0.034805373	1.472670879	1.919925040
C	-0.034770154	2.892105367	1.913622034
C	2.425225685	1.472667767	1.919273180
C	2.425249378	2.892087336	1.914874669
C	1.195280385	3.602272518	1.912547902
C	1.195305562	5.021943376	1.909483480
C	-0.034709730	5.732304454	1.908125378
C	-0.034681654	7.151956947	1.907457648
C	4.885203100	1.472683497	1.915941556
C	4.885233604	2.892085241	1.915159850
C	3.655280567	3.602277649	1.914472608
C	3.655305589	5.021924762	1.912895983
C	2.425318338	5.732324430	1.910833728
C	2.425327549	7.151947794	1.909901119
C	1.195326933	7.862467529	1.908497904
C	1.195299111	9.281926694	1.909291616
C	-0.034704480	9.992878370	1.910931909
C	-0.034766762	11.412355280	1.915238551
C	7.345189428	1.472699501	1.914901361
C	7.345230364	2.892100750	1.915964096
C	6.115259703	3.602273262	1.916073853
C	6.115293773	5.021908880	1.915981918

C	4.885304490	5.732333925	1.914917546
C	4.885311316	7.151905716	1.914544113
C	3.655326630	7.862471866	1.912659303
C	3.655288727	9.281905315	1.912846110
C	2.425308338	9.992869727	1.911947433
C	2.425236963	11.412339042	1.914694782
C	1.195252618	12.122785928	1.917695893
C	1.195172784	13.542511111	1.923201270
C	-0.034844864	14.252873637	1.927592557
C	-0.034862176	15.672538917	1.929303675
C	9.805184050	1.472711281	1.916373838
C	9.805240090	2.892114139	1.915759400
C	8.575246589	3.602279130	1.916784288
C	8.575298517	5.021912157	1.916537853
C	7.345303724	5.732320362	1.917218261
C	7.345318554	7.151896836	1.916874894
C	6.115318433	7.862446782	1.916684909
C	6.115282224	9.281892332	1.916423230
C	4.885297352	9.992849128	1.915686537
C	4.885231255	11.412303562	1.915916828
C	3.655252928	12.122772624	1.916752630
C	3.655184647	13.542489685	1.918411881
C	2.425187860	14.252864461	1.922880144
C	2.425162261	15.672536432	1.924244737
C	1.195153091	16.382685331	1.927506699
C	1.195184907	17.802203044	1.922780516

C	12.265171533	1.472697702	1.918038694
C	12.265227313	2.892117353	1.913682593
C	11.035288150	5.021918903	1.912655234
C	11.035288150	5.021918903	1.912655234
C	9.805297381	5.732323436	1.915335303
C	9.805321228	7.151904609	1.914917407
C	8.575311096	7.862425820	1.916802458
C	8.575288180	9.281899690	1.916235034
C	7.345286932	9.992834810	1.917007811
C	7.345241318	11.412281320	1.915749887
C	6.115241891	12.122771807	1.915976624
C	6.115193201	13.542454615	1.914291333
C	4.885181941	14.252843986	1.916326114
C	4.885169638	15.672527608	1.915732420
C	3.655159563	16.382685703	1.919950341
C	3.655184882	17.802195053	1.918320995
C	13.495234066	3.602282377	1.911533431
C	13.495280479	5.021934862	1.908679543
C	12.265280608	5.732319165	1.910250419
C	12.265302488	7.151925278	1.910051770
C	11.035296570	7.862442312	1.913140641
C	11.035277739	9.281906526	1.913463760
C	9.805272526	9.992844946	1.915525873
C	9.805230853	11.412303721	1.915437069
C	8.575232387	12.122770850	1.915228428
C	8.575197181	13.542457203	1.913511496

C	7.345191822	14.252832339	1.912752564
C	7.345170546	15.672515266	1.911703505
C	6.115159323	16.382694555	1.913264542
C	6.115179123	17.802182862	1.914003888
C	13.495290456	7.862456405	1.908885064
C	13.495271858	9.281921653	1.910156451
C	12.265259103	9.992871420	1.913159868
C	12.265217415	11.412335982	11.412335982
C	11.035203302	12.122775304	1.917184065
C	11.035173941	13.542494857	1.918647507
C	9.805174577	14.252836732	1.915630967
C	9.805160605	15.672523024	1.915161203
C	8.575167125	16.382701031	1.913155490
C	8.575176528	17.802187194	1.914412272
C	13.495203986	12.122784681	1.918963882
C	13.495159959	13.542512588	1.924308800
C	12.265132020	14.252853433	1.923667594
C	12.265133153	15.672544859	1.923967150
C	11.035151352	16.382700575	1.919340216
C	11.035178218	17.802213677	1.917798513
C	13.495128271	16.382694656	1.926933375
C	13.495167745	17.802220363	1.921767178
C	-0.053119341	-0.016253009	5.390680718
C	-0.053105323	1.403618187	5.380078809
C	2.407393310	-0.015779332	5.377525178
C	2.407836299	1.403788461	5.365391961

C	1.177449909	2.113485499	2.113485499
C	1.177312154	3.533109921	5.359478306
C	-0.053333856	4.243138512	5.356516738
C	-0.053274704	5.663039838	5.349462224
C	4.867387520	1.403984090	5.346597118
C	4.867387520	1.403984090	5.346597118
C	3.637561276	2.113674797	5.347642161
C	3.637448669	3.533010203	5.337895336
C	2.407727453	4.243199630	5.345639012
C	2.407543308	5.662801196	5.338739316
C	1.177187271	6.373492251	5.345017575
C	1.177141228	7.792808584	5.342433329
C	-0.053048468	8.503746699	5.349784472
C	-0.053038304	9.923264030	5.355990786
C	7.326938179	-0.015792329	5.360992296
C	7.327065746	1.404218537	5.348613652
C	6.097249415	2.113819079	5.339514812
C	6.097516413	3.533207797	5.327379040
C	4.867143826	4.243293703	5.327119605
C	4.866670780	5.662867536	5.319445812
C	3.636835247	6.373277403	5.325786932
C	3.636456862	7.792679905	5.322171099
C	2.406983468	8.503931842	5.332552337
C	2.406856909	9.922978328	5.337590114
C	1.177077932	10.633598885	5.354151692
C	1.176949351	12.052730512	5.367633968

C	-0.053313902	12.763368212	5.380017614
C	-0.053349676	14.183284558	5.390068651
C	9.786844812	-0.015912441	5.365247665
C	9.787273767	1.403873828	5.352577672
C	8.557098825	2.114198939	5.343485073
C	7.327458718	4.243186010	5.320501217
C	7.327214388	5.662974010	5.310164350
C	6.096708916	6.373417919	5.310306518
C	6.096261453	7.792853621	5.308205546
C	4.866178216	8.503834949	5.315454354
C	4.866145027	9.923001075	5.322537934
C	3.636245105	10.633431382	5.333988453
C	3.636485089	12.052855840	5.348238301
C	2.407082054	12.763230007	5.365819362
C	2.407038281	14.183113578	5.378700354
C	1.176927565	14.893697029	5.390219208
C	1.177159679	16.313401109	5.389680246
C	12.246485984	-0.016031527	5.378727788
C	12.246434548	1.403747678	5.365539782
C	11.017092958	2.113778016	5.348863377
C	11.017321580	3.533369985	5.334012425
C	9.787500208	4.243488297	5.323549348
C	9.787426970	5.662980838	5.315378771
C	8.557395325	6.373419517	5.308863447
C	8.556911111	7.792887603	5.309462456
C	7.326398320	8.503825558	5.310006560

C	7.326164530	9.923284743	5.319141470
C	6.096223229	10.633584998	5.326576234
C	6.096511051	12.052442700	5.342227755
C	4.866291043	12.763169030	5.352456267
C	4.866708927	14.183046227	5.364940400
C	3.636997414	14.893757389	5.374345712
C	3.637300367	16.313765583	5.372153917
C	13.476600121	2.113861629	5.368176488
C	13.476511115	3.533174376	5.353984103
C	12.246759741	4.243484067	5.338063390
C	12.246631045	5.662846973	5.332237515
C	11.017209602	6.373585555	5.322600496
C	11.016781792	7.792995894	5.325144388
C	9.786965572	8.503935262	5.319235488
C	9.786458582	9.923165684	5.325694388
C	8.556130818	10.633650212	5.326549854
C	8.556339347	12.052840628	5.337751073
C	7.326533656	12.762879095	5.347830543
C	7.326627066	14.182942099	5.359949653
C	6.096774877	14.893754664	5.365345682
C	6.096970683	16.313616611	5.363674166
C	13.476531180	6.373435820	5.342773004
C	13.476458387	7.792758884	5.344616431
C	12.246111563	8.503975201	5.338816338
C	12.245879937	9.923214896	5.344751710
C	11.016171943	10.633788204	5.337190996

C	11.016018831	12.052956584	5.345954429
C	9.786207884	12.763069084	5.345378430
C	9.786391451	14.182438575	5.359164965
C	8.556591521	14.893344951	5.363199643
C	8.556766274	16.313201780	5.364963454
C	13.476320347	10.633670316	5.359398483
C	13.476132301	12.053091844	5.369944705
C	12.245760611	12.763206408	5.364594982
C	12.246151975	14.182835863	5.376017518
C	11.016265918	14.893155293	5.371234498
C	11.016526986	16.313117776	5.373425921
C	13.476388291	14.893485396	5.389332872
C	13.476596998	16.313162176	5.389636488
Zn	7.325524097	7.081727339	8.694158139
N	5.728160184	8.198502797	8.733446986
N	6.747778581	10.346930622	8.764754283
N	4.062071697	6.491316857	8.780693742
N	8.471464350	8.737568961	8.734404674
N	10.572321804	7.676924094	8.777252172
N	6.158223723	5.429401512	8.734466879
N	7.879533481	3.825175588	8.761646778
N	8.907127995	5.974707525	8.734232174
C	5.716499652	9.550437932	8.754818766
C	4.459385948	7.733115077	8.762614709
C	4.355379873	9.986494838	8.790750311
C	3.573486289	8.847474561	8.795094200

C	3.779205239	11.221942841	8.827249104
C	2.213767686	8.927012223	8.835311076
C	8.002993711	9.993682943	8.770688676
C	4.818946113	5.430302071	8.781089183
C	10.257531529	10.092747620	8.842832998
C	9.119729758	10.881753620	8.834812366
C	9.811549314	8.736062697	8.779048075
C	11.495629230	10.659936791	8.902604694
C	9.209881477	12.239018525	8.881973625
C	5.507565495	3.283068078	8.833974053
C	4.369693513	4.073969879	8.843566810
C	6.623261489	4.173676505	8.768833565
C	5.414181069	1.924988642	8.879680771
C	3.129638364	3.513334606	8.901060193
C	10.177785616	6.434333424	8.761911666
C	10.261846251	4.181143665	8.789513481
C	11.055959183	5.311817854	8.794137116
C	8.908681778	4.623623414	8.754045538
C	10.812610047	2.937341038	8.827056939
C	12.413208391	5.211293919	8.836670534
C	1.644373910	10.162667361	8.863535016
C	2.419519931	11.295436412	8.859037325
C	4.169399736	1.371715451	8.921916648
C	3.044262867	2.152565902	8.932669081
C	12.960667473	3.963343017	8.863187171
C	12.171344438	2.842158043	8.857690280

C	10.452059111	12.798667443	8.923594618
C	11.579882411	12.020059944	8.934892338
H	2.241885583	4.142876506	8.913436307
H	6.311699695	1.311029381	8.879100225
H	10.172725418	2.059285585	8.835186489
H	13.027235291	6.107269816	8.852923608
H	12.383727338	10.034144818	8.916870295
H	8.306556650	12.844051236	8.881053918
H	4.396303992	12.117247894	8.831617746
H	1.615946858	8.017615747	8.846615658
H	2.070609835	1.669579590	8.957425689
H	4.064947028	0.289861104	8.937548791
H	12.639521113	1.862995493	8.887578589
H	14.039839630	3.848340298	8.897574171
H	12.553722871	12.502538450	8.961034673
H	10.556098639	13.879664828	8.938631280
H	1.931096113	12.266584022	8.888252925
H	0.561992269	10.259318890	8.896195307

Notes and references

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