

Supplementary Materials to “Hole Hopping in Dimers of N,N' Di(1-Naphthyl)-N,N'-Diphenyl-4,4'-Diamine (α -NPD): A Theoretical Study” by I. D. Krysko, A. Y. Freidzon, and A. A. Bagaturyants

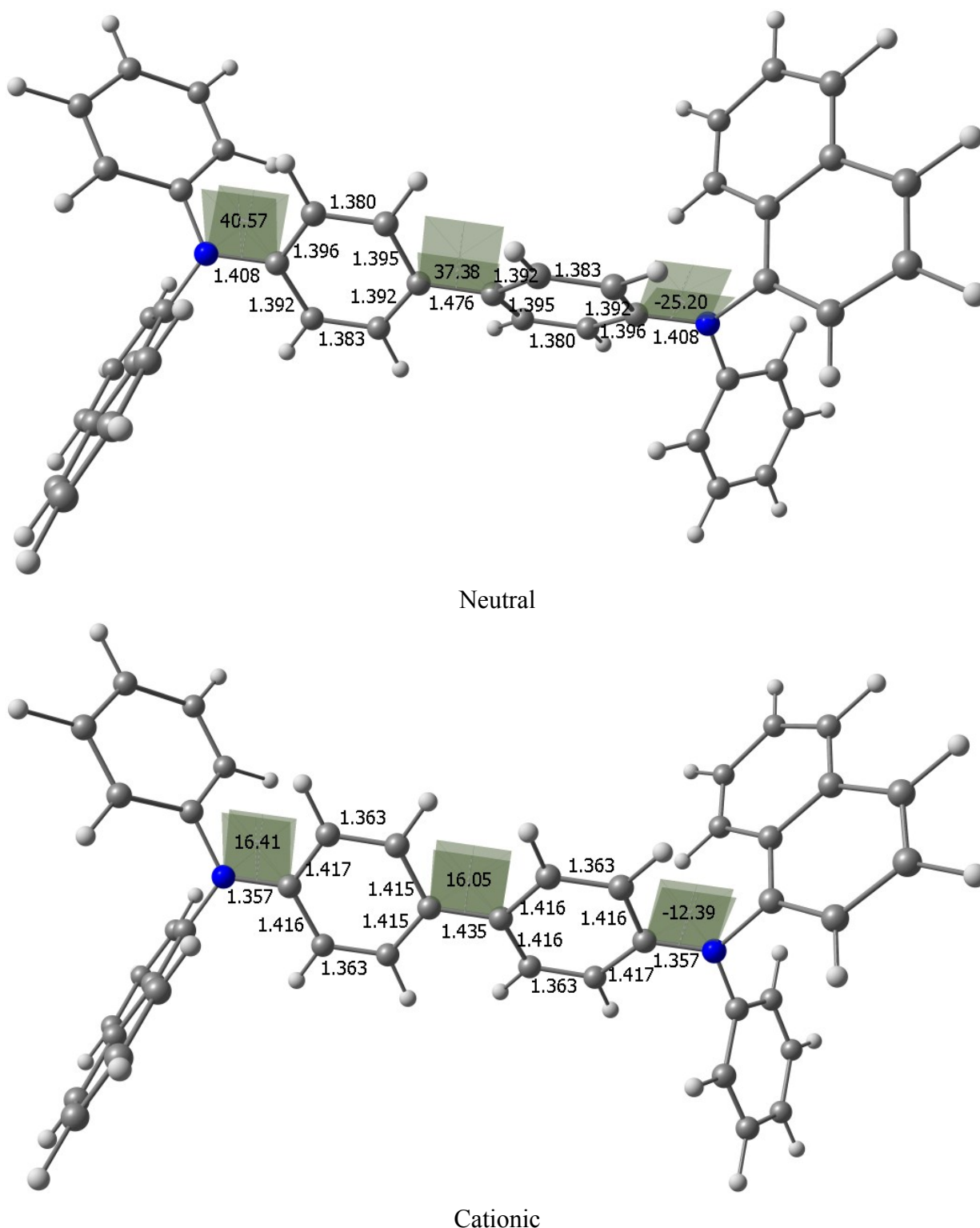


Figure S1. Geometrical parameters of the neutral and cationic monomers

Table S1. Hopping integrals in model dimers calculated as state splitting near the conical intersection point and as Energy Splitting in Dimer (ESID) in the geometry near the conical intersection point (Cartesian coordinates given below)

Dimer	$2V$, eV	ESID, eV
A	0.004	0.014
B	0.006	0.019
C	0.004	0.024
D	0.005	0.003
E	0.003	0.003
A (4.8 Å)	0.023	0.030
A (5 Å)	0.012	0.022

Cartesian coordinates of the optimized monomers (neutral and cationic) and dimers of α -NPD
(near-conical intersection point of the reaction coordinate)

Neutral:

N	4.758419324	4.765060574	-0.038887681
C	4.347900388	3.550501603	0.555077970
C	4.960541168	3.057463309	1.704914398
C	4.533377898	1.866066280	2.266671158
C	3.481737658	1.157895112	1.707661821
C	2.863035244	1.653068709	0.569883901
C	3.294325786	2.833268881	-0.008180904
C	3.756610305	5.709347772	-0.392036657
C	3.659529062	6.175156870	-1.735677689
C	2.656716482	7.128262233	-2.052915890
C	1.769128669	7.569063328	-1.045017882
C	1.869818982	7.085592735	0.225352098
C	2.874585279	6.157776358	0.553768100
H	5.769886114	3.607623882	2.153510721
H	5.019400474	1.498683570	3.156195631
H	3.149217439	0.234297296	2.151779898
H	2.045979675	1.112449073	0.119934650
H	2.818810081	3.208272812	-0.898838058
H	2.957765944	5.787793044	1.562137229
H	1.007208128	8.287963785	-1.300996812
H	1.189199831	7.419262601	0.991349362
C	2.555918404	7.600082779	-3.382161552
C	3.396006004	7.142683011	-4.353659817
C	4.507971158	5.711406617	-2.767636059
C	4.378351309	6.182530661	-4.041751060
H	1.795263843	8.328637082	-3.614650676
H	3.308592165	7.509202123	-5.363476696
H	5.258936109	4.977705074	-2.534759919
H	5.030825845	5.817144971	-4.817881282
C	6.109073643	5.163836745	-0.025472077
C	7.127093774	4.234195742	-0.242648790
C	8.449889466	4.628389145	-0.250181055
C	8.816988876	5.961836481	-0.065855139
C	6.463998033	6.496318077	0.165138686
C	7.791721918	6.882260493	0.135368403
H	6.876349842	3.198161337	-0.394632863
H	9.214857005	3.882304772	-0.391781896
H	5.696702198	7.233871031	0.325242786
H	8.031943808	7.925901811	0.257439451
C	10.232779876	6.379577592	-0.085999786
C	10.709013788	7.370556420	0.773195363
C	12.032298169	7.762413199	0.763446526
C	12.938350297	7.184586622	-0.126862438
C	12.474253905	6.195873799	-0.989955938
H	10.038841532	7.818689980	1.488783620
H	12.373798954	8.514159143	1.454641237
N	14.292967665	7.568833952	-0.120834862
C	15.280780965	6.647274976	-0.561776705
C	15.964012899	6.880785500	-1.724774000

C	16.953044759	5.988337110	-2.175853124
C	17.236619374	4.860074787	-1.465722130
C	16.557729326	4.583697243	-0.257138967
C	15.573785707	5.489975263	0.217264615
H	15.735412380	7.764960173	-2.296268292
H	17.474633632	6.199945272	-3.094818099
H	17.986990022	4.166891292	-1.811139511
C	14.938840157	5.219478948	1.451648573
C	15.252185558	4.100242730	2.166789840
C	16.214946312	3.190518798	1.687591124
C	16.852030593	3.430384067	0.506337490
H	14.203374287	5.910873792	1.822658442
H	14.761500422	3.909741256	3.107307065
H	16.448800533	2.308373537	2.261072557
C	14.666772097	8.923042088	0.031505766
C	13.894951013	9.955712490	-0.495984807
C	14.288367008	11.273447762	-0.333928159
C	15.460818489	11.583802337	0.336072216
C	16.236358319	10.556584852	0.851781442
C	15.842311233	9.238368214	0.709961576
H	16.441160315	8.444048977	1.122865042
H	15.765814299	12.610330409	0.454543942
H	17.149357413	10.780922754	1.379406048
H	13.678685005	12.060251378	-0.748270793
C	11.149001025	5.801790479	-0.960978568
H	13.152141695	5.741370284	-1.691618652
H	10.815345437	5.051203870	-1.658997813
H	17.596785644	2.743240798	0.136739861
H	12.989281179	9.723421210	-1.029580583

Cation radical:

N	4.810438061	4.777901820	-0.016428970
C	4.401412468	3.433065034	0.238839409
C	4.838409626	2.774677334	1.382208862
C	4.412472650	1.481322238	1.633612529
C	3.543893601	0.850169354	0.756937485
C	3.099971548	1.516971395	-0.375299809
C	3.525394643	2.807194543	-0.638620977
C	3.766197534	5.750182838	-0.167404744
C	3.521887130	6.336127666	-1.440216185
C	2.471793632	7.286845439	-1.539255205
C	1.705889651	7.603206374	-0.394524407
C	1.956922052	7.004092224	0.804523511
C	2.998868735	6.067336464	0.917683533
H	5.497948321	3.276946200	2.070403218
H	4.749562598	0.973618860	2.521908022
H	3.209039816	-0.153630886	0.957782921
H	2.422481663	1.031347335	-1.057508424
H	3.182735877	3.329747046	-1.515624651
H	3.199478156	5.592569598	1.863703482
H	0.910387725	8.324728733	-0.487392084
H	1.365721293	7.245368421	1.671516470

C	2.206598309	7.887273696	-2.791555303
C	2.936095382	7.557163651	-3.894886086
C	4.256430888	6.008790248	-2.603854382
C	3.967975220	6.603455284	-3.798018705
H	1.408888423	8.609299184	-2.858921945
H	2.722723393	8.018206671	-4.844716508
H	5.043761974	5.277109934	-2.546672216
H	4.531831469	6.339666928	-4.677507002
C	6.117307066	5.142404905	-0.055900805
C	7.151115129	4.182925351	-0.188616174
C	8.457230174	4.569001096	-0.245110050
C	8.850003988	5.926160796	-0.160319652
C	6.492155561	6.506008178	0.011065663
C	7.804511451	6.871321509	-0.029745653
H	6.900610686	3.140554897	-0.257182308
H	9.203586387	3.800119338	-0.335360040
H	5.730564771	7.257965027	0.104827553
H	8.034523734	7.920840901	0.014254562
C	10.228400011	6.322457581	-0.208185642
C	10.651958252	7.608241929	0.206312724
C	11.958186362	7.995088048	0.162967790
C	12.959115715	7.113341264	-0.313625755
C	12.553770302	5.820611094	-0.723913118
H	9.937877987	8.299642577	0.616766643
H	12.237887195	8.968784545	0.520841858
N	14.265464215	7.479204049	-0.356780375
C	15.299430985	6.506224480	-0.562026246
C	15.975372566	6.503660522	-1.749638298
C	17.004139354	5.574577926	-1.982257746
C	17.334388342	4.667602711	-1.018888239
C	16.664700915	4.652882474	0.225420231
C	15.628821104	5.591362165	0.476113651
H	15.712057209	7.220915843	-2.509130485
H	17.522643641	5.584129556	-2.925881000
H	18.120536965	3.950616146	-1.191943252
C	14.993202099	5.582781564	1.739709382
C	15.361165074	4.681742750	2.696595328
C	16.378126344	3.740569502	2.444160114
C	17.013761573	3.730176382	1.238214966
H	14.218904735	6.300242181	1.949975518
H	14.872520842	4.691159727	3.656876386
H	16.654936472	3.035328441	3.209843851
C	14.676762427	8.844301062	-0.272382845
C	14.154800343	9.787353309	-1.150098323
C	14.582877122	11.102158407	-1.077644425
C	15.536801556	11.474796221	-0.143529033
C	16.064136946	10.526954166	0.720933832
C	15.637901121	9.211821684	0.660612168
H	16.044642460	8.471819849	1.328923479
H	15.872607771	12.496955728	-0.093496658
H	16.807577072	10.811455225	1.446586555
H	14.180387565	11.831070254	-1.761150213

C	11.243471825	5.449956398	-0.669173864
H	13.287830577	5.136370190	-1.107988696
H	10.983843798	4.472018131	-1.033111484
H	17.799899459	3.019596784	1.040105890
H	13.428389253	9.488577427	-1.887609206

Dimer A:

N	10.314039997	0.635894582	-0.296036405
C	10.978857896	1.437464622	-1.262578832
C	10.823470139	2.820176579	-1.272459036
C	11.493314177	3.584642552	-2.212847991
C	12.332838048	2.983736699	-3.137378408
C	12.496471306	1.606808005	-3.117810571
C	11.821975791	0.833597399	-2.189789755
C	11.112527486	-0.268735307	0.467708257
C	10.890117004	-1.671506236	0.366778800
C	11.703942642	-2.536341197	1.144773187
C	12.712806625	-1.990281001	1.970334475
C	12.914512693	-0.643056247	2.025082102
C	12.104158797	0.223596092	1.270500978
H	10.184192694	3.290452458	-0.544392435
H	11.367580930	4.654989204	-2.211854841
H	12.857008302	3.582220024	-3.863688207
H	13.146610113	1.129532798	-3.832510554
H	11.944534008	-0.236283787	-2.177678020
H	12.260335918	1.288416742	1.319229187
H	13.326387657	-2.659791198	2.551479046
H	13.688046437	-0.231439669	2.651649942
C	11.496119897	-3.932454973	1.060746754
C	10.539093684	-4.449985824	0.239231344
C	9.912190613	-2.238801366	-0.483011968
C	9.743623088	-3.591680382	-0.544648849
H	12.115524127	-4.583046276	1.657310948
H	10.391511596	-5.515773203	0.181749727
H	9.302018220	-1.591811479	-1.088487749
H	8.997388222	-4.009490076	-1.200302723
C	8.983425215	0.831179363	0.025796074
C	8.079605782	1.361070704	-0.912065242
C	6.757260607	1.533045139	-0.590407963
C	6.247770578	1.189101359	0.673357763
C	8.486500349	0.476896829	1.290121877
C	7.160113297	0.653772391	1.596428980
H	8.430657390	1.633406318	-1.891483183
H	6.102698525	1.960327122	-1.330744004
H	9.153697318	0.061761573	2.024162982
H	6.816452018	0.350610765	2.570622410
C	4.843319735	1.375029381	1.007830614
C	4.422038445	1.575469112	2.333724897
C	3.101147772	1.753030036	2.657595209
C	2.108635235	1.728191880	1.662023039
C	2.515361440	1.532417672	0.332760190
H	5.153552449	1.634836473	3.121494615

H	2.821004339	1.932454492	3.680467989
N	0.776385175	1.921048673	1.977839330
C	-0.150346272	2.321517072	0.968166821
C	-1.106717137	1.439454111	0.546349368
C	-2.040847774	1.808402632	-0.437607734
C	-1.997220223	3.053889880	-0.990393125
C	-1.029367853	3.995465878	-0.573053113
C	-0.090773617	3.638687865	0.430611170
H	-1.138365868	0.452812911	0.977814037
H	-2.783484568	1.095502759	-0.754799958
H	-2.706719413	3.340990534	-1.749764341
C	0.844290843	4.607639828	0.863255324
C	0.854274453	5.858254418	0.316936203
C	-0.065437301	6.208107325	-0.690869949
C	-0.984715678	5.298036253	-1.121342332
H	1.548791697	4.351817891	1.635120349
H	1.569778315	6.587296167	0.660260209
H	-0.042612213	7.198599230	-1.114438039
C	0.246373642	1.559820904	3.245452842
C	0.571646165	0.341832541	3.834494614
C	0.031384514	0.001734511	5.063229654
C	-0.846203611	0.860148589	5.706345347
C	-1.179003172	2.068082300	5.111929767
C	-0.634897121	2.421840753	3.890132180
H	-0.888391082	3.362391113	3.430813892
H	-1.269237014	0.589446243	6.659346959
H	-1.859890415	2.743174848	5.603755181
H	0.287841214	-0.944524113	5.510774165
C	3.842421299	1.365400033	0.023297697
H	1.775450323	1.495306429	-0.446755065
H	4.107605461	1.184272004	-1.004295428
H	-1.698344342	5.560687139	-1.885904277
H	1.240378397	-0.333994272	3.328581918
N	-0.696451771	-1.776172930	-1.722584990
C	-0.123643284	-1.284430385	-2.926238320
C	-0.382448784	0.011080149	-3.363053341
C	0.198955058	0.476344263	-4.530499068
C	1.052294007	-0.334719163	-5.261685381
C	1.319182698	-1.621171725	-4.817949419
C	0.733464708	-2.098961573	-3.659232811
C	0.190715806	-2.340191612	-0.756117179
C	0.071057399	-3.713085045	-0.397976225
C	0.970968992	-4.233981607	0.568643060
C	1.961005385	-3.392947380	1.125445612
C	2.062768671	-2.088562519	0.742142146
C	1.166964731	-1.558395333	-0.203146801
H	-1.032457313	0.648352699	-2.787476554
H	-0.006549161	1.481603068	-4.860157286
H	1.507530123	0.032665082	-6.166257967
H	1.980970582	-2.260113993	-5.379249457
H	0.936178988	-3.099800699	-3.317120363
H	1.244425942	-0.525921651	-0.500815417

H	2.640633055	-3.803928896	1.854592389
H	2.822251441	-1.452425074	1.165090124
C	0.865871767	-5.594306688	0.939930898
C	-0.074510801	-6.403884224	0.375227645
C	-0.887297526	-4.580018214	-0.972685593
C	-0.955809997	-5.889911573	-0.595903125
H	1.550360299	-5.982128207	1.677419475
H	-0.143494666	-7.439556969	0.664382513
H	-1.562588982	-4.197872036	-1.717972741
H	-1.688462732	-6.539468895	-1.046023857
C	-2.027420937	-1.570651026	-1.408690401
C	-2.996849823	-1.423003478	-2.416493004
C	-4.317835016	-1.239084099	-2.095857457
C	-4.760973027	-1.193819154	-0.762980489
C	-2.457243037	-1.534218991	-0.072690460
C	-3.783096627	-1.350792239	0.232069264
H	-2.697510124	-1.455301794	-3.448973504
H	-5.025055930	-1.110413728	-2.897356916
H	-1.738532853	-1.652624606	0.718347593
H	-4.072920919	-1.348866721	1.268920775
C	-6.164415757	-0.997451646	-0.430246671
C	-6.558433543	-0.411981441	0.785329029
C	-7.878291026	-0.221791016	1.106227543
C	-8.896383965	-0.622555063	0.223200384
C	-8.517326345	-1.205572385	-0.996266546
H	-5.809472231	-0.060586002	1.474383852
H	-8.139403134	0.256076352	2.033807970
N	-10.228955884	-0.421148493	0.532249519
C	-11.213727095	-0.419979223	-0.501611683
C	-12.113996753	-1.447138870	-0.572800626
C	-13.102992762	-1.468067188	-1.571972051
C	-13.169700353	-0.462780059	-2.490482489
C	-12.262575885	0.619964941	-2.442893416
C	-11.269437015	0.659023410	-1.429135649
H	-12.058448955	-2.245368711	0.148564624
H	-13.799655386	-2.288837579	-1.608628495
H	-13.921742029	-0.476008079	-3.262958292
C	-10.396600613	1.770558421	-1.373990838
C	-10.497050357	2.780641201	-2.286264774
C	-11.470975518	2.734860012	-3.302785245
C	-12.332424229	1.680708079	-3.375233596
H	-9.651485994	1.817100254	-0.599277990
H	-9.827841889	3.623344241	-2.228553127
H	-11.535382031	3.538662525	-4.017458910
C	-10.691136545	-0.392268037	1.875304506
C	-10.257676883	-1.337447401	2.799975674
C	-10.732852903	-1.301564627	4.100075400
C	-11.651940878	-0.338578474	4.485521121
C	-12.092316571	0.594918857	3.559323917
C	-11.614116565	0.574401589	2.261290952
H	-11.951283994	1.302727722	1.543149936
H	-12.023963172	-0.317543893	5.496266417

H	-12.806301419	1.348384185	3.848746203
H	-10.392668457	-2.038854040	4.808701097
C	-7.191664281	-1.380828971	-1.307160444
H	-9.276067342	-1.533799629	-1.684066452
H	-6.945480523	-1.862723971	-2.237885108
H	-13.086927673	1.642398002	-4.144690037
H	-9.556186569	-2.096830168	2.498079190

Dimer B:

N	9.717031226	0.127112128	-0.430172811
C	10.258870953	0.836736908	-1.536214200
C	9.634169206	1.979794465	-2.025039619
C	10.187380734	2.666810052	-3.092463836
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C	-8.785952766	-5.595117588	1.908188025
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