Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information For "Locality of Conical Intersections in Semiconductor Nanomaterials"

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Within this document are the Cartesian coordinates for all geometries provided in the text, as well as calculated electronic state energies. All electronic state energies are listed in atomic units and molecular geometries are written in Angstrom.

Silicon Nanocrystal with Single Dangling Bond Defect ($Si_{72}H_{63}$)
E_{S0}(FOMO-CASCI) = -307.29971813
E_{S1}(FOMO-CASCI) = -307.29899551

XYZ Coordinates (Angstrom):

Si	0.0076002773	0.0056878681	2.3708277395
Si	0.0388678163	-0.0271752787	4.7433961007
Si	2.2231615770	0.0460193503	1.5502747400
Si	2.2309883884	0.0643150535	-0.8191592070
Si	-1.0660751180	-1.9621135920	1.6143122203
Si	-1.1177450367	1.9420816251	1.5795860257
Si	-1.1044802497	-1.9183219249	-0.7636832829
Si	-1.1208353745	1.9503635050	-0.8034979572
Si	0.1301609942	-3.8721305426	2.3984874764
Si	3.2514668906	-1.9332589739	2.2374923626
Si	0.1938841260	-3.9748777120	4.7475493911
Si	3.2965035309	-2.2402336536	4.5774371711
Si	1.1580409709	-1.9724038170	5.4960694492
Si	2.3655890295	-4.5148827101	1.5266609144
Si	-2.2569459388	0.0077989005	-1.5797008146
Si	1.1153121864	2.0032212908	-1.6160278910
Si	1.1360977731	-1.9045997432	-1.5552269043
Si	-2.2511119269	3.8774231123	-1.5941466582
Si	-2.2501982494	3.8445155187	-3.9618836196
Si	-3.2920693497	1.9173367229	-4.8158434595
Si	-0.0928976178	3.7689470538	-4.8972864592
Si	-2.2405977541	-0.0088411470	-3.9540753312
Si	1.1066941992	1.9557245775	-3.9887394326
Si	-0.0006399813	-0.0063687198	-4.6770408721
Si	2.3185666224	-3.8253030086	-0.8165559723
Si	1.1236974130	-1.9327837569	-3.9235026057
Si	4.4958219790	-3.8050515651	-1.7201730349
Si	1.1355267989	-5.7329503979	-1.6297484031
Si	0.0065071529	-3.8673699020	-4.6944504959
Si	3.3412608519	-1.9179429734	-4.7380920371
Si	1.1533283460	-5.7808705948	-3.9757829612
Si	4.4533693174	-3.8700665055	-4.0619187771
Si	-2.1949866705	0.0001916491	5.5231179376
Si	1.1284092509	1.9269302186	5.5090838101

Si	-3.3322328673	1.9562066057	2.4007970846
Si	-0.0237825128	3.8758716038	2.3893989698
Si	-4.4575359232	3.8719699829	-0.7385149150
Si	-1.1484542182	5.7960154540	-0.7560246118
Si	-1.1731836457	5.7859797714	1.5991457948
Si	-0.0237546411	3.8378079940	4.7535862745
Si	-3.2837909112	1.9457248444	4.7646212878
Si	-4.4248951462	3.8996783235	1.6152457231
Si	-2.2309368513	3.8895113349	5.5538717009
Si	-3.3566633100	5.8107704624	2.4557169506
Si	-3.3302852151	5.8197767295	4.8004680732
Si	-3.2028966949	-1.9481115614	-4.8772995077
Si	-4.4790396219	0.0235634836	-0.7441136282
Si	-2.2451393375	-3.8397815971	-1.5492493921
Si	-2.2134434203	-3.8462197707	-3.9151866920
Si	-0.8836131062	-5.8534195153	1.5537186624
Si	-1.0657385351	-5.7445897805	-0.7845133043
Si	-3.3038699787	-1.9449390977	2.4087992635
Si	-4.3733830466	0.0025995986	1.6076930327
Si	-5.6731813604	-1.8985494286	-1.3957598948
Si	-4.6061115241	-3.7353471865	1.5981350578
Si	-4.4727910760	-3.8151922249	-0.7483541829
Si	3.3527705657	-5.8108167116	-4.7878257736
Si	3.3613180139	1.9594758698	2.3734002379
Si	2.2145542231	3.9343855207	-0.7782135698
Si	2.1840045051	3.8467346744	1.5780379879
Si	5.5596252189	-1.8869396835	-0.8781057869
Si	4.4330166157	0.0269401859	-3.9732774914
Si	4.4654595593	0.0797696298	-1.6059128755
Si	5.5664383491	2.1185873056	1.5530678480
Si	4.4843011713	4.0193135439	-1.4035332562
Si	5.5559306464	2.0161316189	-0.7953483948
Si	3.3374274601	2.0774630361	4.7257763447
Si	-3.4698393347	-1.8138707218	4.7520130667
Si	-5.7067968479	1.9610214077	-1.2849404613
Si	1.1164724177	5.9340999367	-1.3612258894
Si	5.4567684811	-2.2195877210	1.4342453542
Si	3.2727534258	1.8417241656	-4.9073993858
H	3.3462226780	-5.8757488699	-6.2611360495
H	4.0575605465	-6.9974131540	-4.2653154696
H	0.4228055487	-6.9830750383	-4.4318051355
H	5.8422355555	-3.8476807973	-4.5691446044
H	5.2102235349	-4.9867614124	-1.1908601692
H	3.2799795304	-1.8593258373	-6.2154633257
H	1.8291913638	-6.9283667253	-1.1067286987
H	-0.0154167020	-3.8158962458	-6.1729377676
H	5.8327736596	0.0170082342	-4.4530938889
H	6.9723057679	-1.8441731863	-1.3124276253
H	-1.7585878451	-6.9531071087	-1.2812313213
H	-2.9032559171	-5.0686477947	-4.3807009684
H	-2.1844335052	-6.0562979790	2.2059284518

H	-0.0150511567	-6.9901711361	1.9069712129
H	5.8870691918	-3.5932552577	1.7485806756
H	6.3022436936	-1.2959688665	2.2096049735
H	6.9452124135	2.0191709680	-1.3015674417
H	4.0005769785	3.1068692531	-4.7317832803
H	3.1327486158	1.6046783296	-6.3575156110
H	-0.0016345125	-0.0220192205	-6.1575893667
H	-4.6671523728	-1.9458092559	-4.7508424050
H	-2.8772262187	-1.9489619377	-6.3169131662
H	-5.1555624499	-5.0268163064	-1.2509614564
H	-4.7102404438	5.8521220266	5.3196531593
H	-2.6175022376	7.0185907091	5.2819160604
H	-4.0566770432	7.0082452598	1.9460349560
H	-2.2052634557	3.8626155354	7.0317085293
H	0.7059525339	5.0379451000	5.2204600205
H	-0.4382938287	6.9799115442	2.0708599351
H	-5.8250762583	3.8570148611	2.0895292391
H	-4.6828899720	1.9096361080	5.2445886612
H	-5.1430227770	5.0896711229	-1.2222828390
H	-1.8732032858	6.9925601329	-1.2366616102
H	1.1242799976	1.9194311872	6.9886279421
H	-2.1651284030	0.0089185832	7.0020961362
H	-5.7634210639	-0.0330270519	2.1141907802
H	1.2504730830	-1.9317926481	6.9711231104
H	2.8891912936	5.0488410902	2.0776013812
H	-2.9546652615	5.0520111482	-4.4453260526
H	-6.8950611115	1.9573002189	-0.4079777109
H	-6.1781871239	1.9567266320	-2.6774575875
H	-3.0851761039	-3.0750013580	5.4004318088
H	-4.8856594205	-1.5534437255	5.0779006530
H	3.9015265915	3.3834234507	5.1201352677
H	4.1801146605	1.0226093507	5.3116647741
H	1.3022243533	6.2609355322	-2.7832235299
H	1.7278151306	7.0146696742	-0.5620914299
H	-6.9431511311	-1.8982149961	-0.6415467730
H	-5.9946246761	-1.8668044024	-2.8305640124
H	-6.0076561482	-3.4240960396	1.9446632936
H	-4.2523785059	-5.0110984204	2.2369987743
H	-1.1261220549	-4.2683107540	5.3193262742
H	1.1095911072	-5.0671351093	5.1264859133
H	4.3286681026	-1.3456454741	5.1233086827
H	3.7317896234	-3.6251365369	4.8298737253
H	6.0826344429	3.4463483278	1.9415354394
H	6.4345468528	1.0977060015	2.1602235847
H	4.6428605522	4.3511312951	-2.8268045320
H	5.1054058241	5.1007843207	-0.6119526705
H	-0.2471736554	3.5114448810	-6.3440957393
H	-4.7330203240	1.8914639066	-4.5237388865
H	0.6437048613	5.0321223019	-4.7344943837
H	-3.1272290280	1.9148404136	-6.2833083349

Pristine Silicon Nanocrystal ($Si_{72}H_{63}$)
E_{S0}(FOMO-CASCI) = -307.81162398
E_{S1}(FOMO-CASCI) = -307.81076034

XYZ Coordinates (Angstrom):

Si	0.0188827288	-0.0799628441	2.3719069454
Si	0.0591693409	-0.1045630605	4.7358721923
Si	2.2693204915	-0.0055126145	1.5633204522
Si	2.2549482744	0.0070674596	-0.8043294241
Si	-1.2017115857	-1.9880846587	1.6245173959
Si	-1.0962314360	1.8831196612	1.5852662116
Si	-1.1370227659	-1.9617975324	-0.7529379309
Si	-1.1068295430	1.9114538364	-0.7949612790
Si	-0.3957709276	-4.0097895592	2.4974123336
Si	3.5722618432	-1.8169724335	2.3000267826
Si	0.0953618409	-4.0668888670	4.7746073900
Si	3.3738664839	-2.2976871555	4.6049661267
Si	1.1786163900	-2.0814447687	5.4257504336
Si	2.5742064139	-4.6149305692	1.5026443891
Si	-2.2619842253	-0.0180560191	-1.5724877225
Si	1.1344583621	1.9510175775	-1.6024151952
Si	1.1315547486	-1.9616180064	-1.5160276582
Si	-2.2236462855	3.8510253917	-1.5856850517
Si	-2.2378630093	3.8311800029	-3.9519934753
Si	-3.2518910744	1.9100154297	-4.8496749916
Si	-0.0767404377	3.7654531573	-4.8683851019
Si	-2.2518679963	-0.0217616558	-3.9444216574
Si	1.1065168168	1.9321795849	-3.9761376893
Si	-0.0090337804	-0.0289084978	-4.6515870177
Si	2.3430886635	-3.8916230359	-0.8323276196
Si	1.1119437384	-1.9544476962	-3.8943179760
Si	4.4940612437	-3.8303049719	-1.7959587214
Si	1.1365053149	-5.7679463065	-1.6639740057
Si	-0.0099471238	-3.8756817760	-4.6927112881
Si	3.3139040310	-1.9055929627	-4.7513794976
Si	1.1484137335	-5.7978120765	-4.0147183965
Si	4.4450964263	-3.8597276418	-4.1378567109
Si	-2.1771619348	-0.0355910125	5.5222672550
Si	1.1377371725	1.8533537540	5.5128790931
Si	-3.3183796228	1.9470958859	2.4045729867
Si	-0.0096382133	3.8226575109	2.3945478776
Si	-4.4334917773	3.8640985752	-0.7388069676
Si	-1.1088572161	5.7662916501	-0.7512538855
Si	-1.1355560161	5.7479445972	1.6045981709
Si	-0.0024450860	3.7772720889	4.7598645687
Si	-3.2547413260	1.9251402977	4.7703794610
Si	-4.3927719119	3.8992950060	1.6157554980
Si	-2.2074019810	3.8706855010	5.5575581849
Si	-3.3199349486	5.8075688781	2.4512436116
Si	-3.3052104843	5.8014538430	4.7960049532

Si	-3.2198830493	-1.9512980455	-4.8831087844
Si	-4.4949850507	0.0248131441	-0.7558671320
Si	-2.2659352862	-3.8785064700	-1.5631698796
Si	-2.2369005477	-3.8584323523	-3.9294450494
Si	-1.0417615572	-6.0204450579	1.5009975108
Si	-1.0771710019	-5.7957097788	-0.8404397736
Si	-3.4422493520	-1.8828363552	2.4113856935
Si	-4.4586877780	0.0598753530	1.5972787070
Si	-5.6830380034	-1.9150298820	-1.3800700532
Si	-4.6304606628	-3.7515254753	1.6134326553
Si	-4.4873154322	-3.8384462263	-0.7337239138
Si	3.3131215825	-5.7608292304	-4.9198951590
Si	3.3648217663	1.9442679401	2.3871655263
Si	2.2367588386	3.8863016411	-0.7733927775
Si	2.1929968355	3.8173230634	1.5822286207
Si	5.6096160460	-1.9353449765	-0.9552840410
Si	4.4250197224	0.0263501544	-3.9858386129
Si	4.4843737857	0.0373854778	-1.6181867378
Si	5.5671427079	2.1371226888	1.5689918499
Si	4.5039464647	3.9574042905	-1.4186077614
Si	5.5745821777	1.9649446404	-0.7787210825
Si	3.3406764949	2.0782330094	4.7373665995
Si	-3.5306613103	-1.7967784992	4.7611485377
Si	-5.6841071020	1.9700038116	-1.3468915214
Si	1.1576330737	5.8986754428	-1.3530204477
Si	5.7227199771	-2.1080602865	1.3822965968
Si	3.2566487848	1.8280877733	-4.9283870517
H	3.2100966722	-5.6985221014	-6.3903542808
H	4.0513496408	-6.9838073862	-4.5539690591
H	0.4178013177	-6.9949523078	-4.4837265940
H	5.8196476039	-3.8213514078	-4.6793271694
H	5.2137153016	-5.0300451362	-1.3133251805
H	3.2017935923	-1.8073489709	-6.2234008930
H	1.8071759295	-6.9860036852	-1.1509521880
H	-0.0268197266	-3.7967124892	-6.1706226330
H	5.8215080140	0.0039649608	-4.4746830895
H	6.9865180247	-1.8745916197	-1.4918268515
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H	-2.9239807882	-5.0769232788	-4.4104830494
H	-2.3468880404	-6.5154218279	1.9662936970
H	-0.0354466263	-7.0364545493	1.8666719975
H	6.2165344438	-3.4310660632	1.7949566639
H	6.6308245831	-1.0993676916	1.9509845292
H	6.9703170534	1.9621876306	-1.2680550737
H	3.9759489366	3.1044774312	-4.7990228662
H	3.0813668478	1.5437220032	-6.3666304496
H	-0.0057614005	-0.0544897545	-6.1318057445
H	-4.6849069306	-1.9448419232	-4.7536446296
H	-2.8894088240	-1.9417758226	-6.3228937021
H	-5.1889930763	-5.0435144706	-1.2258718955
H	-4.6908744468	5.8219794030	5.3026239233

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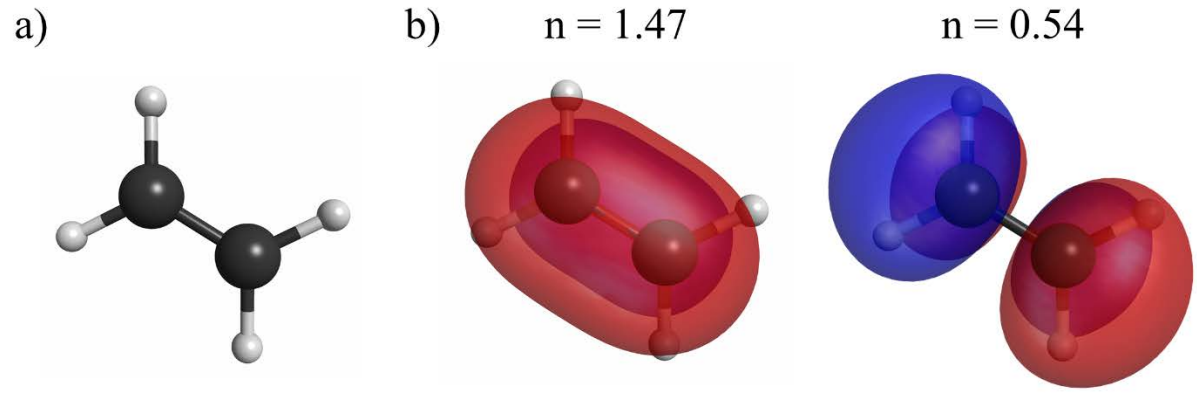
H	-4.0072759817	7.0137598658	1.9437214856
H	-2.1926753605	3.8501085967	7.0357516397
H	0.7501507448	4.9615713772	5.2286180937
H	-0.3781607438	6.9260895943	2.0810245837
H	-5.7884925486	3.8575669461	2.1027945233
H	-4.6514632014	1.8781286249	5.2555521883
H	-5.1087920982	5.0877818934	-1.2234711266
H	-1.8272038941	6.9678088524	-1.2299057188
H	1.1205066121	1.8393620627	6.9922546858
H	-2.1414733263	-0.0183781771	7.0015523210
H	-5.8608684231	0.1114191479	2.0696233683
H	1.2869559449	-2.0486577077	6.9018641932
H	2.8796020399	5.0291108879	2.0822766504
H	-2.9480986995	5.0400934160	-4.4222291135
H	-6.9206015877	1.9706366121	-0.5394141024
H	-6.0735805974	1.9843397373	-2.7643953531
H	-3.1713746930	-3.0886591741	5.3658628615
H	-4.9216981638	-1.4798422047	5.1438391334
H	3.8185791248	3.4254913007	5.1065885136
H	4.2490603357	1.0877493475	5.3393921975
H	1.3541569260	6.2412716927	-2.7697513907
H	1.7755733628	6.9677980581	-0.5425949074
H	-6.9505010691	-1.9148182920	-0.6210812754
H	-6.0179778093	-1.9028224362	-2.8115247525
H	-6.0533469734	-3.5638336247	1.9612800331
H	-4.1594483032	-4.9807383219	2.2680348544
H	-1.0891621793	-4.2954857168	5.6200610805
H	1.0397355950	-5.1750093920	5.0126132748
H	4.3112754421	-1.3840639962	5.2861786046
H	3.8372286404	-3.6761115200	4.8494494201
H	6.0220957767	3.5026229682	1.8992564058
H	6.4734387436	1.1918310777	2.2375860394
H	4.6397071708	4.2395734076	-2.8550495990
H	5.1388194401	5.0627138704	-0.6730811094
H	-0.2073263523	3.5346456373	-6.3213094271
H	-4.7110674918	1.8975886617	-4.6702197631
H	0.6643114850	5.0211222961	-4.6760529597
H	-2.9736465456	1.8999390981	-6.3002643924
H	4.0611755912	-4.8856377279	1.3841936859

Linear Polyenes

Ethylene Ground State

Figure SP1: a) Ground state minimum energy geometry of ethylene optimized at the B3LYP/6-31G** level of theory and verified with a harmonic frequency calculation. b) Fractionally occupied state averaged natural orbitals (SANOs) at the ground state geometry, calculated at the state averaged complete active space self-consistent field method with an active space of two electrons in two orbitals, averaging over the first two electronic states (SA2-CASSCF(2/2)) using the 6-31G** basis set. Orbitals in this figure were generated using an iso value of 0.05.



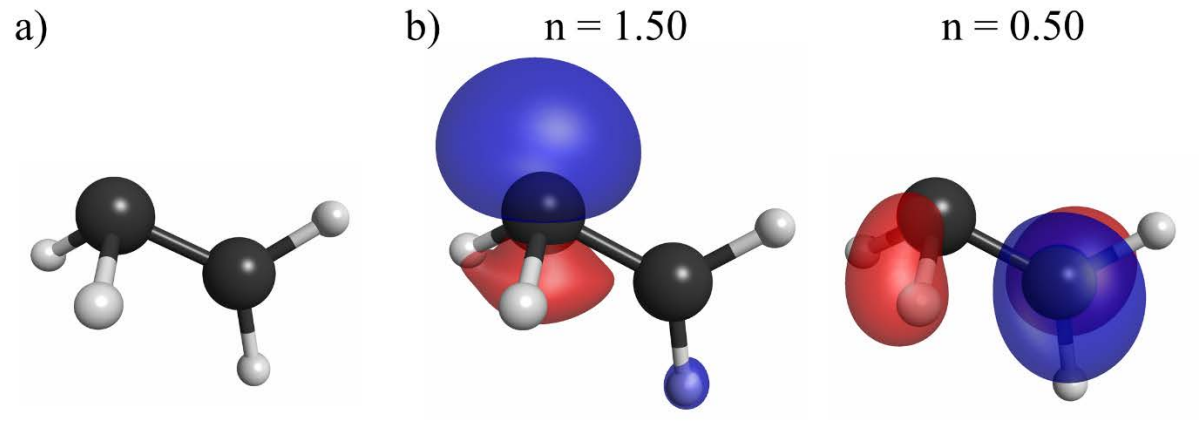
E_{S0}(B3LYP) = -78.53378941
E_{S0}(SA-CASSCF) = -78.05666217
E_{S1}(SA-CASSCF) = -77.67911571

XYZ Coordinates (Angstrom):

C	0.03299228	-0.11889318	0.00907007
C	-0.00991525	0.06922682	1.32592408
H	0.95299243	0.00203732	-0.55742249
H	0.87311328	0.35206457	1.89348898
H	-0.92975570	-0.05162988	1.89261881
H	-0.84995105	-0.40179666	-0.55867946

Ethylene Minimal Energy Conical Intersection (MECI)

Figure SP2: a) Ethylene twisted and pyramidalized conical intersection (CI) optimized at the SA2-CASSCF(2/2)/6-31G** level of theory. b) Fractionally occupied SANOs calculated at the same geometry and level of theory. Orbitals in this figure were generated using an iso value of 0.10.



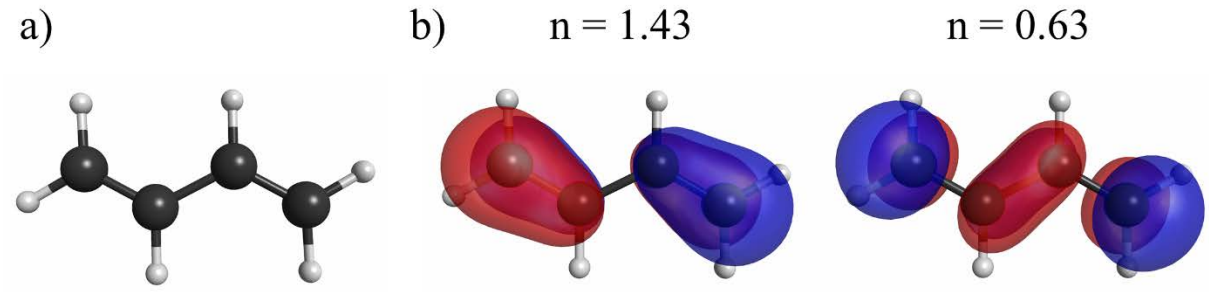
E_{S0}(SA-CASSCF) = -77.84962276
E_{S1}(SA-CASSCF) = -77.84903694

XYZ Coordinates (Angstrom):

C	-1.85664260	0.01491828	-0.40730906
C	-0.61846185	-0.22001444	0.17102659
H	0.34368208	-0.10652418	-0.33115253
H	-1.98519969	0.80636662	-1.13417888
H	-1.39500201	-0.79568094	-1.11483955
H	-0.52955925	-0.69955528	1.14192414

Butadiene Ground State

Figure SP3: a) Ground state minimum energy geometry of butadiene optimized at the B3LYP/6-31G** level of theory and verified with a harmonic frequency calculation. b) Fractionally occupied SANOs at the ground state geometry, calculated at the SA2-CASSCF(4/4)/6-31G** level of theory. Orbitals in this figure were generated using an iso value of 0.05.



E_{S0}(B3LYP) = -155.88846909
E_{S0}(SA-CASSCF) = -154.98072248
E_{S1}(SA-CASSCF) = -154.73391159

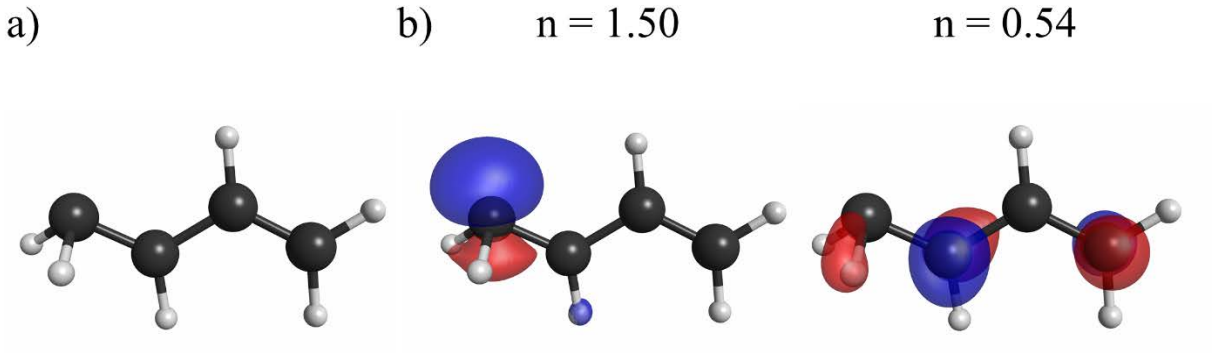
XYZ Coordinates (Angstrom):

C	-0.02492233	-0.09587989	0.07776005
C	-0.04703417	0.04898262	1.41050393
C	1.19048270	-0.10657506	-0.72694275
C	1.21417076	-0.25031786	-2.05974994

H	2.14529229	-0.25225987	-2.61795870
H	0.29908422	-0.37176253	-2.63472615
H	2.12893785	0.01227956	-0.18469299
H	-0.96388915	-0.21526532	-0.46354129
H	-0.97738167	0.05080022	1.96985654
H	0.86902348	0.17171112	1.98386629

Butadiene MECI

Figure SP4: a) Butadiene twisted and pyramidalized CI optimized at the SA2-CASSCF(4/4)/6-31G** level of theory. b) Fractionally occupied SANOs calculated at the same geometry and level of theory. Orbitals in this figure were generated using an iso value of 0.10.



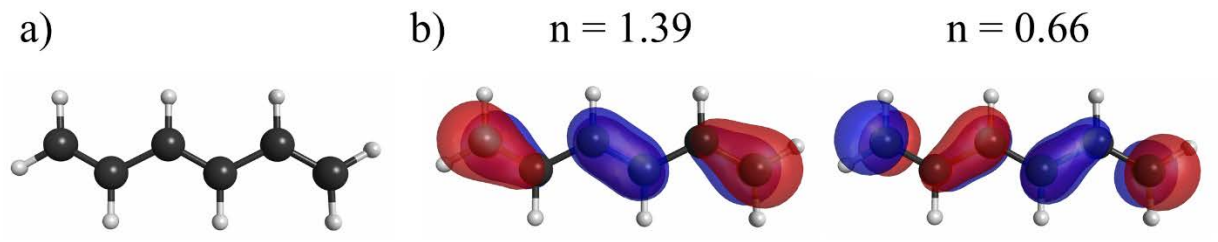
E_{S0}(SA-CASSCF) = -154.78271115
E_{S1}(SA-CASSCF) = -154.78209231

XYZ Coordinates (Angstrom):

C	-1.88087237	-0.02421518	-0.39643210
C	-0.62328744	-0.21704181	0.17726409
C	0.60920984	-0.00281282	-0.55347943
C	1.81088054	0.07257514	0.06295758
H	-1.86741924	0.81892288	0.40707180
H	-2.71840596	-0.56950217	0.03487498
H	-0.45688996	-0.40949029	1.24239540
H	0.50714326	0.11126217	-1.61594069
H	1.90287828	-0.01803994	1.13088524
H	2.71676278	0.23834209	-0.48959684

Hexatriene Ground State

Figure SP5: a) Ground state minimum energy geometry of hexatriene optimized at the B3LYP/6-31G** level of theory and verified with a harmonic frequency calculation. b) Fractionally occupied SANOs at the ground state geometry, calculated at the SA2-CASSCF(6/6)/6-31G** level of theory. Orbitals in this figure were generated using an iso value of 0.05.



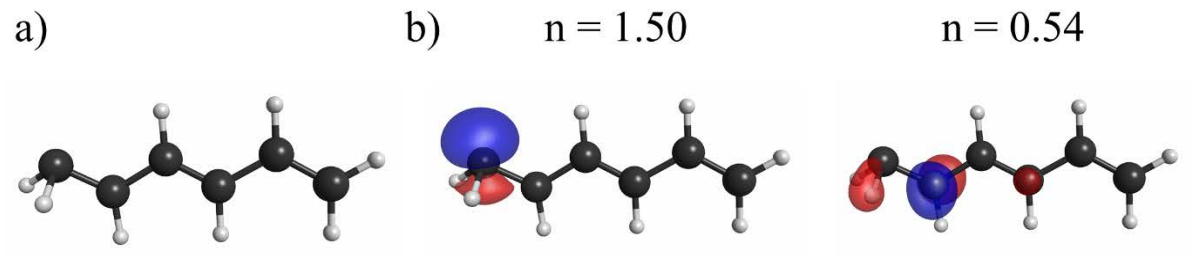
E_{S0}(B3LYP) = -233.24497274
E_{S0}(SA-CASSCF) = -231.90035365
E_{S1}(SA-CASSCF) = -231.69561170

XYZ Coordinates (Angstrom):

C	-0.08131535	0.07691485	1.44833053
C	-0.03367677	-0.11202062	0.11924094
C	1.18401833	-0.10105863	-0.66863810
C	1.22773302	-0.28932846	-2.00720990
C	2.44558889	-0.27813769	-2.79498200
H	0.29583875	-0.46302766	-2.54689656
H	2.11597936	0.07302443	-0.12916277
H	-0.96189792	-0.28665364	-0.42572471
H	-1.01953430	0.06019692	1.99359842
H	0.82001319	0.25534638	2.02993645
C	2.49326477	-0.46585077	-4.12418803
H	3.37373750	-0.10359523	-2.24980511
H	3.43148268	-0.44854229	-4.66942350
H	1.59193287	-0.64360961	-4.70608970

Hexatriene MECI

Figure SP6: a) Hexatriene twisted and pyramidalized CI optimized at the SA2-CASSCF(6/6)/6-31G** level of theory. b) Fractionally occupied SANOs calculated at the same geometry and level of theory. Orbitals in this figure were generated using an iso value of 0.10.



E_{S0}(SA-CASSCF) = -231.70524197
E_{S1}(SA-CASSCF) = -231.70505773

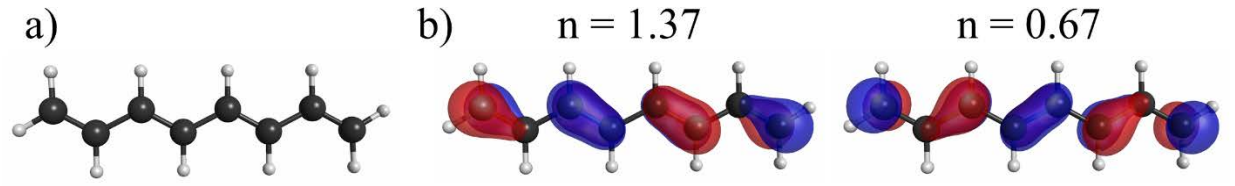
XYZ Coordinates (Angstrom):

C	-1.89475298	-0.04231501	-0.40164122
C	-0.63668853	-0.22968727	0.18863463
C	0.58923763	-0.00518211	-0.54565597

C	1.77660894	0.06710275	0.05752497
H	-1.90597785	0.84985739	0.40853426
H	-2.73861289	-0.57114941	0.05232100
H	-0.48643962	-0.42280018	1.25024068
H	0.49995726	0.11273932	-1.61157393
H	1.83685291	-0.03117397	1.13249111
C	3.03758192	0.29381076	-0.64233303
C	4.21303558	0.38140225	0.00228819
H	2.98637795	0.39393261	-1.71466303
H	5.13840771	0.54972231	-0.51505333
H	4.25614023	0.28413552	1.07116914

Octatetraene Ground State

Figure SP7: a) Ground state minimum energy geometry of octatetraene optimized at the B3LYP/6-31G** level of theory and verified with a harmonic frequency calculation. b) Fractionally occupied SANOs at the ground state geometry, calculated at the SA2-CASSCF(8/8)/6-31G** level of theory. Orbitals in this figure were generated using an iso value of 0.10.

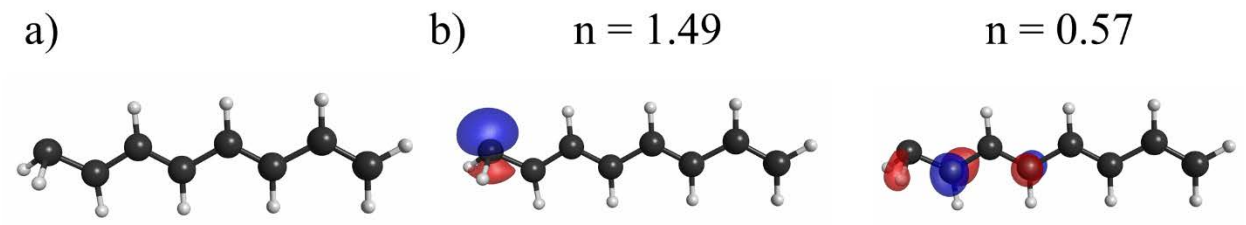


E_{S0}(B3LYP) = -310.60206015
E_{S0}(SA-CASSCF) = -308.81990288
E_{S1}(SA-CASSCF) = -308.64383215
XYZ Coordinates (Angstrom):

C	-0.10685549	0.07753328	1.48243144
C	-0.05146348	-0.11057763	0.15258518
C	1.16904683	-0.09740036	-0.62675749
C	1.22102348	-0.28504835	-1.96873032
C	2.43373770	-0.26917777	-2.74756855
C	2.48619695	-0.45522207	-4.08964540
H	0.29018538	-0.46085863	-2.50978077
H	2.09736631	0.07882004	-0.08168145
H	-0.97665530	-0.28640710	-0.39728958
H	-1.04791263	0.05999074	2.02238684
H	0.79154212	0.25671398	2.06820213
H	3.36478742	-0.09469411	-2.20642535
C	3.70725625	-0.43763705	-4.86797279
H	1.55815161	-0.63013152	-4.63542863
C	3.76458823	-0.62056252	-6.19844163
H	4.63144950	-0.26228039	-4.31625306
H	4.70617662	-0.59733923	-6.73747428
H	2.86735549	-0.80044529	-6.78584930

Octatetraene MECI

Figure SP8: a) Octatetraene twisted and pyramidalized CI optimized at the SA2-CASSCF(8/8)/6-31G** level of theory. b) Fractionally occupied SANOs calculated at the same geometry and level of theory. Orbitals in this figure were generated using an iso value of 0.10.



E_{S0}(SA-CASSCF) = -308.62709659
E_{S1}(SA-CASSCF) = -308.62647274

XYZ Coordinates (Angstrom):

C	0.53436553	-0.01401809	-0.54653490
C	1.74336648	0.06405209	0.07050698
C	2.99882483	0.28699815	-0.63015354
C	4.17448664	0.37715557	-0.01623212
C	-0.68833148	-0.24084303	0.17958772
C	-1.96375418	-0.06438515	-0.40739673
H	-1.91998160	0.83976346	0.40496713
H	-2.80088663	-0.56127799	0.08107849
H	-0.54256481	-0.42160907	1.24540079
H	0.44629440	0.11642311	-1.61100972
H	1.79203093	-0.04123193	1.14263844
H	2.94306779	0.38526523	-1.70182514
C	5.45093393	0.60471010	-0.69512391
H	4.21548557	0.27900594	1.05717087
C	6.62503004	0.68959153	-0.04603165
H	5.42016983	0.70453882	-1.76830077
H	7.55178595	0.85646594	-0.56581265
H	6.67695332	0.59263527	1.02548647

Slab Model of Silicon Nanocrystal with Two Dangling Bond Defects ($Si_{70}H_{68}$)
E_{S0}(FOMO-CASCI) = -302.53903357
E_{S1}(FOMO-CASCI) = -302.53834569

XYZ Coordinates (Angstrom):

Si	-2.5422709268	2.3089075580	-0.0473146060
Si	-0.1859643952	2.3928016834	-0.1490124730
Si	-3.3710301982	4.3018248285	0.9094592593
Si	-3.1815277015	0.4844880756	1.3206970751
Si	0.7375374557	2.7153668288	1.9959907253
Si	-2.4592897189	4.6145852313	3.0659294912
Si	-2.2499121267	0.8073362246	3.4631485018
Si	-0.0996491263	4.7026561048	2.9628902834
Si	-3.0975517326	2.7876003766	4.4339201703
Si	0.1096620020	0.8883881025	3.3650209646
Si	0.6562780717	0.3992374559	-1.1265080065
Si	-5.7207266974	4.2332405229	1.0583722266
Si	-2.3360432382	-1.5047336923	0.3776030510
Si	-5.5263977923	0.3932199087	1.4952598159
Si	0.9430381757	-1.0973328094	2.3971144204
Si	0.9607211387	1.1790027577	5.5381520069
Si	0.7568198169	5.0100939677	5.1355791141
Si	-5.4576684247	2.7119085702	4.5466150903
Si	-2.2051423245	3.0968258049	6.5992090029
Si	-6.3449298279	2.3995884357	2.3919830242
Si	0.1427714119	3.1713752167	6.4672607201
Si	0.0060684596	-1.4095832979	0.2635644322
Si	-3.3962583975	2.0113597452	-2.2210851141
Si	-3.3010187693	6.6004831525	4.0354889132
Si	3.0812075126	2.8114033411	1.7885710703
Si	-6.2688103488	4.7034660076	5.5032492415
Si	-6.5385110764	6.2316915842	1.9791728203
Si	-0.0625831717	6.9968110557	6.0821932032
Si	-3.0669338866	5.0782805683	7.5307709477
Si	3.2852729890	-1.0209321251	2.2241186779
Si	-3.2200897012	-1.8393848967	-1.7741937998
Si	-0.2659086230	0.0870610009	-3.2691504559
Si	3.0063393105	0.4423136102	-1.2589109333
Si	-2.4103578722	6.9136517729	6.2012019016
Si	-5.4139420194	5.0076090292	7.6732315458
Si	-5.6597637724	6.5338660684	4.1408997457
Si	-3.2601612861	8.9003311221	7.1351352079
Si	-6.4554960769	8.5391992451	5.0854630530
Si	-6.2416734067	6.9973504292	8.6036828471
Si	-5.6019896839	8.8078834460	7.2553060678
Si	-2.6121548021	-0.0097217812	-3.1245637142
Si	0.5700067558	-1.8909042426	-4.2454345456
Si	0.8379503499	-3.4000384881	-0.6960314440
Si	3.8457552921	-1.5648524575	-2.1926831391
Si	3.9023221586	0.8058061038	0.8803395358
Si	2.9331811213	-1.7864474384	-4.3491025897

Si	-0.3008773859	-2.2227249397	-6.4027883668
Si	-0.0579512445	-3.7030402119	-2.8467323606
Si	3.1629564374	-3.3986681283	-0.8573033130
Si	6.1862884394	-1.5148781052	-2.3403759934
Si	3.8258481404	-3.7138752926	-5.3774394433
Si	0.8239630395	-5.6723175844	-3.7676313598
Si	-2.4024044093	-3.8447588402	-2.6807190685
Si	4.0731140231	-3.0454771730	1.3208233617
Si	4.0295480783	-5.6642890505	-1.1368740562
Si	-0.0156804949	-6.0323661520	-5.9572736217
Si	3.1697417189	-5.4970684224	-4.0073210291
Si	6.1863174299	-3.7271458668	-5.4556798123
Si	2.8895650696	-4.1108933575	-7.5176560740
Si	6.3050544496	-5.3801323495	-1.9949230192
Si	4.0448121306	-7.5284295593	-4.9180547653
Si	0.5487396882	-4.2023503302	-7.3259089601
Si	0.7646663257	-8.0381403749	-6.8789633146
Si	3.7708778518	-6.0873324781	-8.4436670839
Si	6.9788305181	-3.5162464877	-3.2611915157
Si	6.9932093975	-5.7130807066	-6.4427697864
Si	6.4029069685	-7.5489762865	-5.0868399326
Si	6.1080554685	-6.0036895175	-8.5990555027
Si	3.1040237020	-7.9070048056	-7.1051966684
Si	7.1668684853	-7.3680750248	-2.8595682929
H	0.2020539708	3.5400706619	-1.0007514486
H	-2.9607506296	5.4404613162	0.0577929264
H	0.2877531600	5.8545412630	2.1184051061
H	-5.8415117352	1.5674081739	5.4013764050
H	-5.8998213539	-0.7315287104	2.3755047622
H	-6.1225251767	0.1571708590	0.1656906310
H	-6.2791548728	4.0485964682	-0.2980918494
H	-7.8208221515	2.3507570992	2.4844845065
H	2.2319781840	5.0685250701	5.0569812568
H	-2.6115910469	1.9474197656	7.4366914065
H	0.6932967099	3.3633068845	7.8268005626
H	2.4352487972	1.2265144280	5.4928918535
H	0.5561870334	0.0332512178	6.3761300298
H	0.5719606838	-2.2408932851	3.2591607714
H	-2.7214402682	-2.6443893640	1.2394759289
H	0.3462867570	8.1598095440	5.2702090298
H	0.4836201132	7.1609026088	7.4442312582
H	-2.5071522355	5.2694762812	8.8871063602
H	-2.8997073934	7.7487393809	3.1915781631
H	-7.7462637561	4.6425454328	5.5591044386
H	-8.0123067941	6.1855546232	2.0555704350
H	-6.1497113061	7.3713615118	1.1255315804
H	-5.8077656544	3.8574430519	8.5138659323
H	-5.7006021795	7.1690182785	9.9659767378
H	-7.7129520741	6.9275273346	8.6879331078
H	-2.8447205629	10.0457415200	6.3023149009
H	-2.6979956239	9.0766935456	8.4887172911

H	-7.9307412824	8.5123142474	5.1120824682
H	-6.0269090311	9.6743459027	4.2445202288
H	-2.6389479895	-0.3363144424	4.3183377959
H	-6.1156419066	10.0649921953	7.8396167573
H	-4.6936862604	-1.9265226745	-1.6968942732
H	0.1215714321	1.2287958431	-4.1270628744
H	-2.9500647339	3.1304161409	-3.0743859090
H	-4.8712717719	2.0104066443	-2.1918014626
H	-3.1656593987	-0.2078431623	-4.4814721417
H	3.4398531349	3.9394667408	0.9064296153
H	3.6991103866	3.0390105346	3.1089323563
H	3.8738770546	-0.8595767538	3.5711448829
H	3.3996425171	1.5478538644	-2.1599607014
H	5.3768028367	0.8727509294	0.7922902189
H	0.4093675690	-4.5455671654	0.1370156241
H	3.3227431713	-0.6252542199	-5.1775996697
H	-2.7384330244	-4.9769084945	-1.7953330228
H	-3.0036668940	-4.0977580345	-4.0038345492
H	5.5472923830	-3.0272932629	1.2384370689
H	3.6720032792	-4.1746592372	2.1802329731
H	0.5274300517	-6.8517925777	-2.9302562692
H	0.0511085766	-1.0835667017	-7.2726123150
H	-1.7704449890	-2.3325942554	-6.3408054105
H	-1.4861657083	-6.1037736866	-5.8404448545
H	3.2748823575	-2.9748021584	-8.3810406409
H	6.6312878155	-2.5871748907	-6.2843852909
H	6.9247502865	-5.2111912815	-0.6543960200
H	6.7743337393	-1.3350961429	-1.0004588575
H	6.6201154637	-0.3928882638	-3.1961433783
H	-0.0113909171	-4.4521354220	-8.6706326552
H	8.4573518753	-3.5067082329	-3.3208232301
H	8.4684290898	-5.6520235554	-6.5118201637
H	3.1816371112	-6.3009611033	-9.7834416386
H	6.8139778723	-8.8233315240	-5.7101774584
H	6.5124225797	-4.8723085289	-9.4526633080
H	6.6186712195	-7.2596455298	-9.1796290737
H	3.6890816414	-9.1673029244	-7.6046539714
H	0.2016616577	-8.2330554297	-8.2289369339
H	0.4170690750	-9.1942632660	-6.0353031831
H	8.6409509217	-7.3987175488	-2.8850674172
H	6.6654570611	-8.5316007053	-2.1068586498