

Supplementary Information

Graphene Based Frustrated Lewis Pairs as Bifunctional Catalyst for CO₂ Reduction via Dissociative chemisorption of molecular H₂: A Periodic Density Functional Perspective

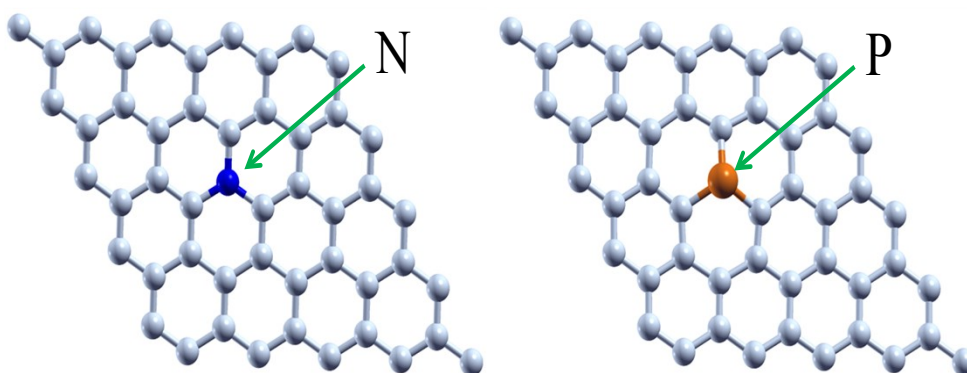
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Supplementary Figure 1. The Optimised conformations of nitrogen and phosphorous doped Nano Graphene.

Supplementary Table 1. The Structural parameters of optimized FLPs

FLPs	NG-B (Å)	NG-Al (Å)	NG-Ga (Å)	NG-In (Å)	PG-B (Å)	PG-Al (Å)	PG-Ga (Å)	PG-In (Å)
Interatomic distance between Fluorine atom on Lewis acid	3.88	3.87	3.87	4.07	3.73	3.86	3.93	4.07
	3.15	3.20	3.17	3.16	3.30	3.27	3.30	3.20
	3.30	3.43	3.45	3.39	3.31	3.48	3.46	3.39

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	3.67	3.66	3.69	3.76	3.93	3.84	3.82	3.90
	4.54	4.49	4.49	4.71	4.35	4.32	4.24	4.32
	3.66	3.75	3.75	3.93	3.63	3.81	3.69	3.85
	3.28	3.22	3.21	3.24	3.38	3.35	3.32	3.30
	3.16	3.24	3.26	3.28	3.33	3.40	3.41	3.32
	3.69	3.72	3.72	3.83	3.83	3.84	3.87	3.89
	4.45	4.37	4.38	4.65	4.43	4.32	4.35	4.44

Supplementary Table 2. The Bader Charge analysis of FLPs w.r.t Lewis acid and base

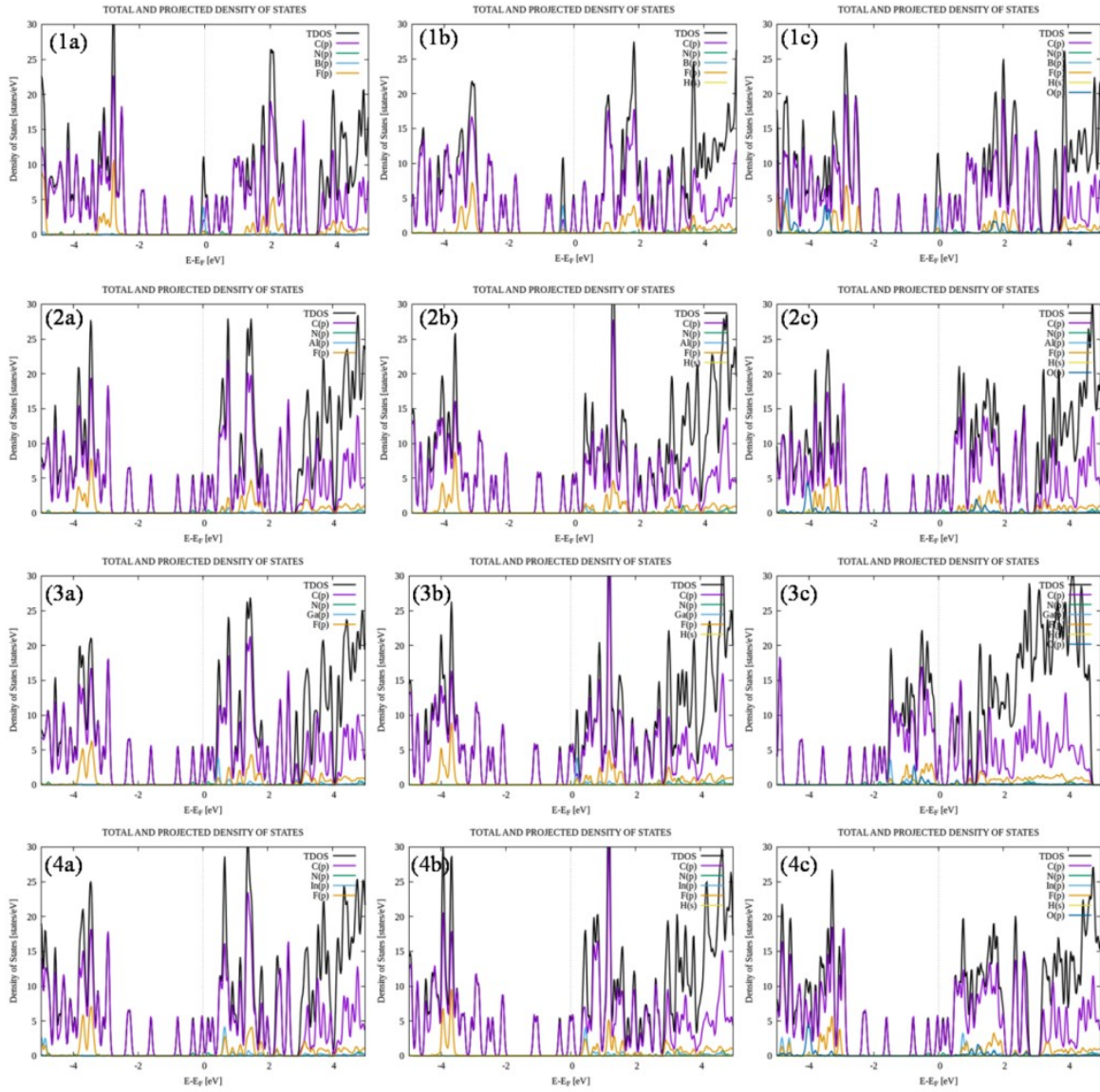
FLPs	Charge on N atom/P atom (e)	Charge on N atom/P atom in uncomplexed Lewis base (e)	B (e)	Al (e)	Ga (e)	In (e)
			Charge on atom in the uncomplexed Lewis acid is given in parenthesis			
NG-B	-1.22	-0.90 (N atom)	1.86 (1.87)			
NG-Al	-1.24			2.23 (2.22)		
NG-Ga	-1.25				1.21 (1.27)	
NG-In	-1.22					1.24 (1.16)
PG-B	1.67	1.59 (P atom)	1.89 (1.87)			
PG-Al	1.62			2.22 (2.22)		
PG-Ga	1.68				1.22 (1.27)	
PG-In	1.60					1.24 (1.16)

Supplementary Table 3. The Bader Charge analysis of NG-B and PG-B FLPs with respect to carbon atoms attached to dopants on N/P doped FLPs. (only NG-B and PG-B FLPs are reported as case study)

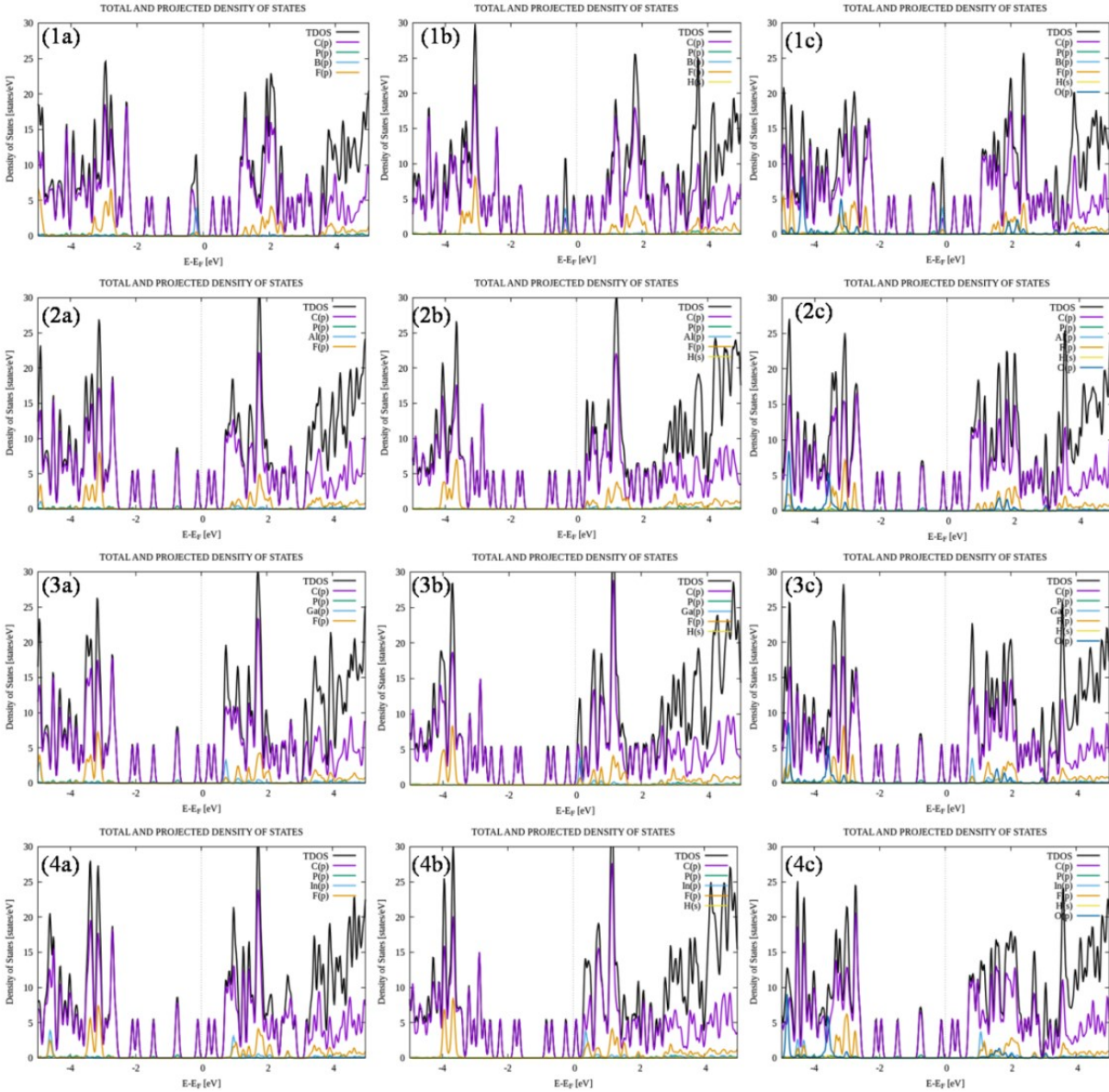
FLPs	Atom	N/P-FLPs (e)	H ₂ —N/P-FLPs (e)	CO ₂ on H ₂ —N/P- FLPs (e)
NG-B	N LB-N (-0.90)	-1.22	-0.95	-1.12
	C (carbon atoms attached to dopant)	0.24	0.05	0.13
		0.43	0.21	0.51
		0.36	0.06	0.34
B LA-B (1.87)	1.86	1.84	1.81	
PG-B	P LB-P (1.59)	1.66	2.43	-0.65
	C (carbon atoms attached to dopant)	-0.70	-0.72	-0.63
		-0.64	-0.55	-0.46
		-0.50	-0.65	-0.60
B LA-B (1.87)	1.89	1.84	1.83	

Supplementary Table 4. The adsorption energy analysis of NG and PG FLPs with respect to (1) Dissociative adsorbed H₂, (2) CO₂ adsorption on H₂ adsorbed surface and (3) HCOOH adsorption (adsorption trend on NG and PG system are used as a reference for 1 and 2)

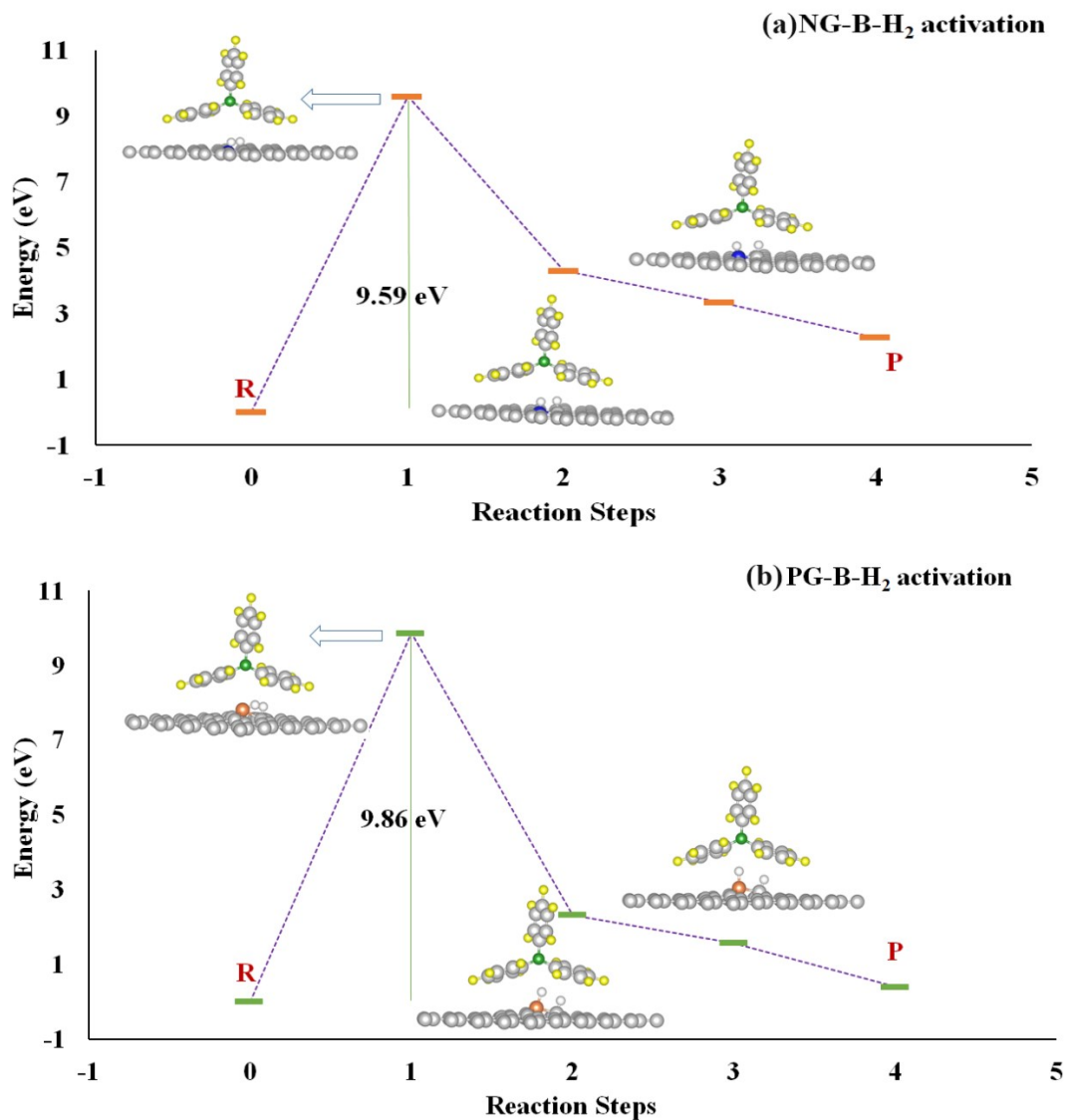
FLPs	1	2	3
	Dissociative adsorption of H ₂ (eV)	CO ₂ adsorption on H ₂ adsorbed surface (eV)	HCOOH adsorption (eV)
NG (N-doped graphene)	-6.48	-0.26	
NG-B	2.27	-0.39	0.62
NG-Al	2.14	-0.33	0.54
NG-Ga	2.15	-0.39	0.51
NG-In	2.12	-0.32	0.63
PG (P-doped graphene)	-6.14	-0.23	
PG-B	0.40	0.10	0.57
PG-Al	0.55	-0.08	0.57
PG-Ga	0.45	-0.09	0.51
PG-In	0.44	-0.13	0.50



Supplementary Figure 2. Total and partial density of states of N-doped FLPs



Supplementary Figure 3. Total and partial density of states of P-doped FLPs



Supplementary Figure 4. The minimum reaction path of H₂ activation on (a) N-doped (NG-B) and (b) P-doped (PG-B) FLP catalysts.

As case study, the potential of (a) N-doped (NG-B) and (b) P-doped (PG-B) FLP catalysts for the H₂ activation has been discussed in Supplementary Figure 4. Along the reaction steps, reactant (R) at step 0 and product (P) at step 4 represents gaseous hydrogen and dissociative chemisorbed hydrogen in presence of catalyst, respectively. NEB calculation is performed by generating 3 steps in between these reactant and product to confirm the activation energy barrier and pathway of the reduction reaction. Both the catalysts shows a very high activation energy barrier of 9.59 and 9.86 eV at reaction step 1, respectively. Along the reaction steps from 1 to 3, the hydrogen atoms distance gradually increases from 0.78 to 1.82 Å in N-

doped (NG-B), and from 0.73 to 2.24 Å in P-doped (PG-B) FLP catalysts, respectively. Owing to strong interaction between the Lewis pair's centers, which increases the activation barrier for H₂ activation.

Coordinates of Optimized Structures

1. NG-N doped graphene Structure (Lewis base)

C N

1.0000000000000000		
13.0000000000000000	0.0000000000000000	0.0000000000000000
6.4992140000000000	11.2587840000000000	0.0000000000000000
-0.9280290000000000	-0.5634710000000000	19.8624500000000000

49 1

Direct

0.9048200000000000	0.9206010000000000	0.2340680000000000
0.8413530000000000	0.8570990000000000	0.2341270000000000
0.9049150000000000	0.7300890000000000	0.2341450000000000
0.8414340000000000	0.6665800000000000	0.2342330000000000
0.9048590000000000	0.5395770000000000	0.2341450000000000
0.8413540000000000	0.4760890000000000	0.2343550000000000
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0.8412300000000000	0.2855240000000000	0.2341210000000000
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0.8412160000000000	0.0949780000000000	0.2340580000000000
0.7143470000000000	0.9206220000000000	0.2340820000000000
0.6508530000000000	0.8571160000000000	0.2340990000000000
0.7144310000000000	0.7301140000000000	0.2342110000000000
0.6509490000000000	0.6666250000000000	0.2344510000000000
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0.7142960000000000	0.3490870000000000	0.2343300000000000
0.6508810000000000	0.4761190000000000	0.2346400000000000
0.6508320000000000	0.2855530000000000	0.2343370000000000
0.7142590000000000	0.1585330000000000	0.2341380000000000
0.6507410000000000	0.0950010000000000	0.2340790000000000
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0.4602890000000000	0.8570900000000000	0.2339010000000000
0.5239320000000000	0.7301080000000000	0.2342180000000000
0.4604680000000000	0.6665980000000000	0.2344430000000000
0.5238790000000000	0.5395870000000000	0.2346020000000000
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0.4602590000000000	0.2854940000000000	0.2340640000000000
0.5237430000000000	0.1584940000000000	0.2339820000000000
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0.3332890000000000	0.9205450000000000	0.2338030000000000

0.2697690000000000	0.8570540000000000	0.2338240000000000
0.3334410000000000	0.7300740000000000	0.2341330000000000
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0.2698830000000000	0.4760120000000000	0.2340810000000000
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0.0795040000000000	0.6665430000000000	0.2341970000000000
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0.0793740000000000	0.4760150000000000	0.2339410000000000
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0.0792370000000000	0.2854790000000000	0.2337920000000000
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0.0792190000000000	0.0949630000000000	0.2337820000000000
0.4604350000000000	0.4760460000000000	0.2344700000000000

2. Boron doped Lewis acid Structure

C B F

1.0000000000000000		
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0.0000000000000000	11.5046420000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	7.4067110000000000

18 1 15

Direct

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0.3313960000000000	0.8305060000000000	0.4227580000000000
0.3627460000000000	0.7973540000000000	0.5951280000000000
0.4157540000000000	0.6935270000000000	0.6193900000000000
0.6253050000000000	0.4999960000000000	0.5000120000000000
0.6782760000000000	0.4999350000000000	0.3369300000000000
0.7842320000000000	0.4999000000000000	0.3369440000000000
0.8371950000000000	0.4999870000000000	0.5000260000000000

0.7842020000000000	0.5000920000000000	0.6631880000000000
0.6782760000000000	0.5000480000000000	0.6631480000000000
0.4373450000000000	0.3771670000000000	0.5287160000000000
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0.3614470000000000	0.2034980000000000	0.4044500000000000
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0.3543390000000000	0.2393190000000000	0.7256590000000000
0.4072860000000000	0.3431900000000000	0.7013970000000000
0.4999980000000000	0.4999960000000000	0.5000120000000000
0.4461010000000000	0.6614790000000000	0.7862250000000000
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0.2801650000000000	0.9310050000000000	0.3991980000000000
0.3227160000000000	0.7918780000000000	0.1077870000000000
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0.6270370000000000	0.4998660000000000	0.1790600000000000
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0.9397190000000000	0.5000310000000000	0.5001070000000000
0.8354630000000000	0.5002130000000000	0.8210320000000000
0.6269830000000000	0.5001870000000000	0.8209640000000000
0.4434810000000000	0.3402610000000000	0.2130970000000000
0.3392260000000000	0.1359170000000000	0.2607830000000000
0.2801190000000000	0.0689960000000000	0.6006240000000000
0.3252980000000000	0.2064280000000000	0.8928320000000000
0.4294620000000000	0.4107710000000000	0.8450910000000000

3. NG-B FLP Structure

C N B F

1.0000000000000000		
12.3813999999999000	0.0000000000000000	0.0000000000000000
6.1912510000000000	10.7252910000000000	0.0000000000000000
-1.1663289999999900	-0.7081590000000000	24.9627359999999000

67 1 1 15

Direct

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0.9505451684210410	0.7649580079497060	0.1731701309881140
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0.2924561883931270	0.3347398887324650	0.3104505047463240
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0.3849044299548180	0.6488875096430060	0.5144215366926870
0.4983552552363930	0.5796783563486890	0.5422917854405010
0.6048645430396430	0.4975259054304980	0.5140878102744490
0.5964650529260660	0.4876143395388030	0.4584296318762930
0.4841089388148920	0.4981224584741890	0.1734378189378430
0.4808514670752380	0.5433334303899950	0.3656244879771110
0.2670597185090500	0.7009029723748490	0.4333263465266260
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0.7022669232133760	0.4079832270451950	0.4323607809077440
0.6032169670160720	0.2759657469703870	0.3493113074384140
0.4863044522958100	0.1462332062182160	0.3191144098147010
0.2337553228490380	0.2695969609546990	0.2983537978121820
0.1034230600217310	0.5264160850340600	0.2978607802892970
0.2236642364515860	0.6564667698273000	0.3198827054328880
0.3619465692627370	0.8049171333426530	0.3509339820176850
0.4761776341058990	0.9303975066677810	0.3205227005051230
0.7266430932270470	0.8006210865861190	0.2982026618849000
0.8529775791043650	0.5452591870544900	0.2971560413760640
0.7333749188106780	0.4191555946337190	0.3184469612561150

4. NG-B-H2 FLP Structure

N C F B H

1.0000000000000000		
12.3814000000000000	0.0000000000000000	0.0000000000000000
6.1912510000000000	10.7252910000000000	0.0000000000000000
-1.1663290000000000	-0.7081590000000000	24.9627360000000000

1 67 15 1 2

Direct

0.4841520000000000	0.4981200000000000	0.1734320000000000
0.5506100000000000	0.3652080000000000	0.1734140000000000
0.6832360000000000	0.2990230000000000	0.1732720000000000
0.7513000000000000	0.3645250000000000	0.1731220000000000
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0.3505690000000000	0.7652850000000000	0.1733880000000000
0.5510830000000000	0.7640340000000000	0.1728490000000000
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0.7509040000000000	0.7648980000000000	0.1726810000000000
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0.4842930000000000	0.8978520000000000	0.1730380000000000
0.5509200000000000	0.9647170000000000	0.1730550000000000
0.6843550000000000	0.8980710000000000	0.1729210000000000
0.7508580000000000	0.9646580000000000	0.1732430000000000
0.8840570000000000	0.8981100000000000	0.1732300000000000
0.9506040000000000	0.7649350000000000	0.1731140000000000
0.0840420000000000	0.0980930000000000	0.1732700000000000
0.9507380000000000	0.9647940000000000	0.1734400000000000
0.2267410000000000	0.4648960000000000	0.3103770000000000
0.2926810000000000	0.3346680000000000	0.3105120000000000
0.4209440000000000	0.2718670000000000	0.3221370000000000
0.4792930000000000	0.3407690000000000	0.3368820000000000
0.4161510000000000	0.4713610000000000	0.3384090000000000
0.2899770000000000	0.5303560000000000	0.3226880000000000
0.4845170000000000	0.5536810000000000	0.4290510000000000
0.3791300000000000	0.6326060000000000	0.4588290000000000
0.3843680000000000	0.6483680000000000	0.5143200000000000
0.4978240000000000	0.5796500000000000	0.5422220000000000
0.6045440000000000	0.4976780000000000	0.5140170000000000
0.5965880000000000	0.4876130000000000	0.4583660000000000
0.5445010000000000	0.6084010000000000	0.3372970000000000
0.6686440000000000	0.5456010000000000	0.3213370000000000
0.7314390000000000	0.6087670000000000	0.3096530000000000
0.6673890000000000	0.7391000000000000	0.3104940000000000
0.5410140000000000	0.8050060000000000	0.3227460000000000
0.4834820000000000	0.7387920000000000	0.3369140000000000
0.1035320000000000	0.5263460000000000	0.2978530000000000
0.6030290000000000	0.2768470000000000	0.3501920000000000
0.4863610000000000	0.1462680000000000	0.3191530000000000
0.2339100000000000	0.2695830000000000	0.2983650000000000
0.2236360000000000	0.6564880000000000	0.3198570000000000
0.2670880000000000	0.7008160000000000	0.4333210000000000
0.2811760000000000	0.7296940000000000	0.5408670000000000
0.5038120000000000	0.5924710000000000	0.5958900000000000
0.7139180000000000	0.4293130000000000	0.5405580000000000
0.7026060000000000	0.4082420000000000	0.4322440000000000
0.7333670000000000	0.4191500000000000	0.3184500000000000
0.3619660000000000	0.8048990000000000	0.3509320000000000

0.4761960000000000	0.9303730000000000	0.3205170000000000
0.7266740000000000	0.8006060000000000	0.2982200000000000
0.8529870000000000	0.5452370000000000	0.2971570000000000
0.4808290000000000	0.5434320000000000	0.3655420000000000
0.5366230000000000	0.5508800000000000	0.2145150000000000
0.5029360000000000	0.5151320000000000	0.2115580000000000

5. NG-B-H2 dissociated FLP Structure

N C F B H

1.0000000000000000		
12.381399999999900	0.0000000000000000	0.0000000000000000
6.1912510000000000	10.7252910000000000	0.0000000000000000
-1.1663289999999900	-0.7081590000000000	24.962735999999900

N C F B H

1 67 15 1 2

Direct

0.4815187032594480	0.4962999979116060	0.1933992482701800
0.5523307912237060	0.3611723247461940	0.1750350025746570
0.6833259816496520	0.2989157644261300	0.1733190008800950
0.7512694403823010	0.3656322459811040	0.1733611516796910
0.6871393998595370	0.4966666789352850	0.1757589797693380
0.5551980986591570	0.5696997144192290	0.1949504834795560
0.7502659823217310	0.1651361882088240	0.1705495873238420
0.8839743890791930	0.0982005304594904	0.1701904144504190
0.9507184034300290	0.1646644847318510	0.1700313538846150
0.8840780917456410	0.2981202842055540	0.1701731282428720
0.4838156039212980	0.2983478792329110	0.1727684116364440
0.5507021131477230	0.1646095014234030	0.1702073215782290
0.6838673569139140	0.0981583519717507	0.1701735870611150
0.3500831476335490	0.3645551365255520	0.1732448504968910
0.2838332032534240	0.2982595901518090	0.1707322446917260
0.3504754631799320	0.1647159088640390	0.1701884609900070
0.4837617044317670	0.0982377331464110	0.1700462722772140
0.1501858718600760	0.3646748312684160	0.1688395171388860
0.0840121314819466	0.2979314527115130	0.1688572513718010
0.1505833694520620	0.1649381035176080	0.1698285255418980
0.2837007149901900	0.0985129898161459	0.1700386777334890
0.7505881610972370	0.5642639911195900	0.1714915496657720
0.8838969087348350	0.4977456031691180	0.1683543518705660

0.9505833119609240	0.3646550373516440	0.1687832584579460
0.3466376710287670	0.5667315273297330	0.1746747477220670
0.2837994506888110	0.4981570934040870	0.1719496915071520
0.1500322406746180	0.5649109269863970	0.1685893878355520
0.0836068344024897	0.4978505085905930	0.1678884865828440
0.2844702290826720	0.6977120444272880	0.1731720526988250
0.1507243559802240	0.7645829529592380	0.1701637652569580
0.0836986837432633	0.6980837561491430	0.1688648117949210
0.4822065554231780	0.7017911920304750	0.1761628619819830
0.3512235719882420	0.7657873168694800	0.1736959658888160
0.5499569283523170	0.7652868041829000	0.1725032607864160
0.6842186222061860	0.6985725115334740	0.1724133557424770
0.7502790568487370	0.7645762144471560	0.1701946980255800
0.8839274471614020	0.6979797935457500	0.1687377511167730
0.9503153098336410	0.5646923288648330	0.1677804608804660
0.2837137090572490	0.8986331574169930	0.1707712987351810
0.1502847233882650	0.9651252413098960	0.1701822671372730
0.0838482831622024	0.8983024845560800	0.1701138907323750
0.3504005791698590	0.9651725534386030	0.1702075568774500
0.4835785540784630	0.8985833827506590	0.1702097822297040
0.5506098565316840	0.9649558026003620	0.1699562260911460
0.6838510966747110	0.8983562004306530	0.1700798571416440
0.7506008697635480	0.9646608937136040	0.1700235861175260
0.8838360274477950	0.8981248692978120	0.1699089180949150
0.9501953372864780	0.7648033966570460	0.1689290662621160
0.0838633865418378	0.0982292892824651	0.1699902041824030
0.9505473848139830	0.9648661917325440	0.1700267006992990
0.2270123231070750	0.4655192508348730	0.3105384665688760
0.2930064227039650	0.3351765191033470	0.3106356939572720
0.4212484512453810	0.2720040545089260	0.3224152600680050
0.4799216265451890	0.3405437331113930	0.3371643988109440
0.4170722719210490	0.4714106004600580	0.3382417827416590
0.2905065397910590	0.5307746005682760	0.3226138810548600
0.4843589864467580	0.5523101975572480	0.4296256468620660
0.3787351203572380	0.6313203778801560	0.4591560488077210
0.3839575066755190	0.6471210114303630	0.5145935106839520
0.4974581780100490	0.5785597790242280	0.5425074753416920
0.6044956918090110	0.4967604881767450	0.5144344454570980
0.5966092707615570	0.4867389535821780	0.4588095611923130
0.5459978147363090	0.6081293227090330	0.3392033776886830
0.6711621746223670	0.5452758393372490	0.3244738414567620

0.7330561863539940	0.6082576840035840	0.3112573005210460
0.6679426406577180	0.7386530367274220	0.3110180240058820
0.5415390115292980	0.8045270732523130	0.3232934828542740
0.4840263135109080	0.7385664989839070	0.3377925096617210
0.1039941954936220	0.5265764849923940	0.2980132099631700
0.6032906979372320	0.2765806285647490	0.3510299157615220
0.4862562518851300	0.1465013955650580	0.3193084477982160
0.2341689292052530	0.2703907510666240	0.2984795578489490
0.2246887763246040	0.6568895221172600	0.3199069659528300
0.2670918850918360	0.7005610808297860	0.4334301288657990
0.2810848612230990	0.7296688128619540	0.5409449328193230
0.5037169675362670	0.5923026901256550	0.5960444720888420
0.7139920561048710	0.4288012891762380	0.5409484680509350
0.7025848476501350	0.4082288458021170	0.4325190168518610
0.7357608658611870	0.4186639870685760	0.3223532678281410
0.3620255802145560	0.8047677673713240	0.3509346983122070
0.4766929314871540	0.9296418599007140	0.3206585302767350
0.7261798719668230	0.8004653327639760	0.2981054105637040
0.8534460582845800	0.5451349536539120	0.2973571672276350
0.4814952112598530	0.5428094971803360	0.3664481970265030
0.5643264143717030	0.5793521928654230	0.2390227424929520
0.4736159583177100	0.4893411280401460	0.2341088793466940

6. NG-B-dissociated H2- CO2 FLP Structure

C B F O N H

1.0000000000000000		
12.3813999999999000	0.0000000000000000	0.0000000000000000
6.1912510000000000	10.7252910000000000	0.0000000000000000
-1.1663289999999900	-0.7081590000000000	24.9627359999999000

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Direct

0.6751170000000000	0.5562630000000000	0.3842050000000000
0.5546630000000000	0.6214850000000000	0.4043500000000000
0.4863800000000000	0.7487290000000000	0.3935830000000000
0.5306940000000000	0.8081200000000000	0.3625160000000000
0.6505500000000000	0.7392870000000000	0.3421380000000000
0.7237860000000000	0.6126650000000000	0.3534200000000000
0.4897090000000000	0.5616080000000000	0.4960340000000000
0.3785570000000000	0.6093200000000000	0.5241750000000000

0.3752700000000000	0.6238540000000000	0.5797310000000000
0.4868960000000000	0.5824290000000000	0.6093420000000000
0.6001830000000000	0.5306230000000000	0.5830920000000000
0.5993660000000000	0.5238530000000000	0.5273530000000000
0.4153650000000000	0.5022530000000000	0.4003680000000000
0.4734940000000000	0.3719130000000000	0.3955930000000000
0.4236240000000000	0.3091600000000000	0.3651750000000000
0.3087220000000000	0.3785210000000000	0.3385030000000000
0.2454640000000000	0.5088630000000000	0.3431170000000000
0.2999450000000000	0.5682550000000000	0.3731640000000000
0.5182370000000000	0.5320070000000000	0.2959560000000000
0.5617180000000000	0.5680290000000000	0.1719500000000000
0.6896270000000000	0.4877270000000000	0.1485130000000000
0.7515740000000000	0.5551990000000000	0.1420390000000000
0.6834350000000000	0.6897010000000000	0.1424640000000000
0.5487390000000000	0.7579550000000000	0.1421370000000000
0.4811920000000000	0.6960560000000000	0.1487040000000000
0.7490170000000000	0.7552770000000000	0.1378710000000000
0.8822930000000000	0.6887170000000000	0.1355790000000000
0.9486340000000000	0.5556490000000000	0.1348830000000000
0.8834040000000000	0.4884370000000000	0.1363780000000000
0.6824310000000000	0.8884600000000000	0.1353810000000000
0.7490440000000000	0.9545310000000000	0.1334520000000000
0.8820360000000000	0.8887700000000000	0.1333950000000000
0.9478990000000000	0.7558540000000000	0.1339180000000000
0.4820850000000000	0.8897040000000000	0.1364470000000000
0.5491440000000000	0.9550740000000000	0.1346700000000000
0.7508440000000000	0.3560580000000000	0.1420690000000000
0.8831920000000000	0.2887820000000000	0.1363820000000000
0.9497220000000000	0.3553390000000000	0.1357060000000000
0.9494630000000000	0.1553010000000000	0.1339520000000000
0.8837860000000000	0.0875860000000000	0.1329440000000000
0.7513870000000000	0.1527310000000000	0.1337600000000000
0.6868980000000000	0.2841740000000000	0.1396410000000000
0.6828090000000000	0.0871700000000000	0.1327970000000000
0.5493420000000000	0.1526090000000000	0.1330310000000000
0.4832200000000000	0.2849810000000000	0.1370620000000000
0.5569330000000000	0.3424410000000000	0.1427880000000000
0.4820940000000000	0.0875110000000000	0.1334070000000000
0.3488070000000000	0.1552550000000000	0.1344040000000000
0.2823270000000000	0.2886810000000000	0.1356070000000000

0.3485800000000000	0.3551940000000000	0.1380470000000000
0.1487410000000000	0.3555120000000000	0.1348010000000000
0.0810800000000000	0.4887290000000000	0.1339370000000000
0.1458400000000000	0.5563460000000000	0.1339450000000000
0.2782040000000000	0.4899570000000000	0.1378910000000000
0.0828370000000000	0.2886490000000000	0.1348360000000000
0.1491640000000000	0.1557820000000000	0.1346860000000000
0.2820870000000000	0.0892380000000000	0.1346660000000000
0.0805350000000000	0.6897340000000000	0.1336440000000000
0.1461630000000000	0.7581430000000000	0.1346050000000000
0.2775180000000000	0.6935860000000000	0.1406920000000000
0.3354980000000000	0.5637250000000000	0.1440620000000000
0.3494530000000000	0.7574510000000000	0.1426270000000000
0.2823000000000000	0.8896310000000000	0.1366730000000000
0.1486040000000000	0.9562340000000000	0.1342440000000000
0.0809830000000000	0.8905180000000000	0.1333400000000000
0.3488050000000000	0.9561600000000000	0.1356930000000000
0.9488450000000000	0.9554990000000000	0.1325880000000000
0.0824640000000000	0.0891390000000000	0.1339300000000000
0.4874070000000000	0.5607320000000000	0.4336980000000000
0.2682210000000000	0.6500970000000000	0.4971300000000000
0.2663990000000000	0.6778540000000000	0.6052260000000000
0.4849290000000000	0.5915850000000000	0.6630420000000000
0.7080700000000000	0.4878150000000000	0.6115210000000000
0.7106770000000000	0.4731520000000000	0.5032630000000000
0.3690390000000000	0.8175900000000000	0.4120530000000000
0.4581400000000000	0.9293270000000000	0.3508800000000000
0.6945950000000000	0.7942550000000000	0.3113080000000000
0.8387670000000000	0.5454430000000000	0.3330750000000000
0.7471210000000000	0.4323450000000000	0.3920680000000000
0.1338660000000000	0.5762830000000000	0.3179350000000000
0.2609510000000000	0.3193600000000000	0.3079360000000000
0.4856040000000000	0.1836360000000000	0.3602750000000000
0.5874480000000000	0.3016690000000000	0.4192970000000000
0.2364260000000000	0.6944070000000000	0.3752740000000000
0.6023290000000000	0.4295060000000000	0.2999360000000000
0.4334960000000000	0.6337060000000000	0.2902630000000000
0.4798540000000000	0.4855460000000000	0.1734290000000000
0.4666140000000000	0.4698040000000000	0.2149580000000000
0.5805290000000000	0.5865230000000000	0.2143690000000000

7. NG-B-HCOOH FLP Structure

C N O F B H

1.0000000000000000		
12.3813999999999000	0.0000000000000000	0.0000000000000000
6.1912510000000000	10.7252910000000000	0.0000000000000000
-1.1663289999999900	-0.7081590000000000	24.9627359999999000

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Direct

0.9503838201133160	0.7654599003523130	0.1575784671355890
0.8838227482920630	0.6988965592641260	0.1576763885405350
0.7506489367709440	0.7653854188899480	0.1576433926739910
0.6842129624181610	0.8985825983054110	0.1577711476651390
0.7506651272518890	0.9652271614281850	0.1575958079784340
0.8838356320836550	0.8986486265961680	0.1576572066966240
0.9504144766770470	0.5654578697611560	0.1567227517299340
0.8834966779463220	0.4987092305434540	0.1558987147316060
0.7496416192401200	0.5653990621234490	0.1545096880576300
0.6837804027367460	0.6984844331758270	0.1558101644511390
0.6825646056349190	0.4984137269759060	0.1518059536115480
0.7507016760837580	0.3648025642467410	0.1522688642781060
0.8831130650358290	0.2988459445850980	0.1545198929292830
0.9504316955161650	0.3655349414484990	0.1556103106647710
0.6825997102283550	0.2992592536018770	0.1515599189461970
0.7495794179498100	0.1658118745980060	0.1542975019929850
0.8834283712392560	0.0989558275276564	0.1557949926401100
0.9504131909360630	0.1650829331974350	0.1555753410224430
0.5500077774081300	0.3652596597774020	0.1496689998853930
0.4838169484907110	0.2991888520394170	0.1515641751690100
0.5507783702748240	0.1655865965052590	0.1543145738505280
0.6838461976897870	0.0986921280392671	0.1555702714382850
0.3500594986854370	0.3647411959297220	0.1522278574421820
0.2840664651885760	0.2988146007700910	0.1546200190836470
0.3507814295137830	0.1649933383533940	0.1556184636361030
0.4840288170265140	0.0987515494152074	0.1558406669385350
0.2844141383470380	0.4984990837434540	0.1514780294874950
0.1507441296520090	0.5654956358345740	0.1542565538932480
0.0839380416143628	0.4987512048762360	0.1558213584704000
0.1502267454071150	0.3655300491304030	0.1556328044591400
0.2841677179366930	0.0984838699032332	0.1561300725327140
0.1504988195723670	0.1652619565890160	0.1560481546192800

0.0837568813742812	0.2988684651632300	0.1561369520308660
0.0838211579924740	0.6986082210710450	0.1555599810666640
0.1507585633349690	0.7645864251727470	0.1542665335560520
0.2844206470079430	0.6975244712521160	0.1512999733851070
0.3504734793747420	0.5647569835935470	0.1493946675980250
0.5506235061926380	0.7643691326822270	0.1545663655525480
0.4837771612211020	0.6972261880117480	0.1517200999385160
0.5499531526029660	0.5645845167945170	0.1500450585298140
0.5507093972519350	0.9652226364593370	0.1568280337393790
0.4839778934049180	0.8982688373023640	0.1559172247092210
0.3507398528696860	0.9652519877971650	0.1556180715828850
0.2840086473737670	0.8980006503976180	0.1544827778516620
0.3500294783809170	0.7656055360292140	0.1520666099458510
0.1501454642731090	0.9653327353657390	0.1555201293545740
0.0838976164745819	0.8984509715043260	0.1558002040185530
0.0836933005489017	0.0985672762839851	0.1560539562205000
0.9503507712198970	0.9653681344314000	0.1566861257835880
0.4630773250738000	0.5093888379520160	0.2628861852133330
0.6718149548457470	0.5404582185692220	0.3530225995212240
0.5521802431967200	0.6037392315622040	0.3740721896483880
0.4872030195390090	0.7334134112041570	0.3697828900934610
0.5353740609821690	0.7986598781504410	0.3455239823435320
0.6561638602392310	0.7323346404978360	0.3260295507464850
0.7247292477216200	0.6028682464711950	0.3297003297640210
0.4137161412663030	0.4790795149962470	0.3755428820525860
0.4781902249850890	0.3486983595065920	0.3707779566696230
0.4269107288887250	0.2803571453742730	0.3462195264861360
0.3031976262321310	0.3432099006463110	0.3273119529240240
0.2345004687098780	0.4732275251579070	0.3318541153321470
0.2912284073562650	0.5383445457452150	0.3547822397699770
0.4894148846162730	0.5523581078886770	0.4667719127884010
0.3804987774759910	0.6125036681166500	0.4966136409224650
0.3827587282839100	0.6285646303320610	0.5520902431362200
0.4977207772665730	0.5775273505351670	0.5797722814513080
0.6086645691757980	0.5140784294957380	0.5517322673891150
0.6028142087377610	0.5052384746876180	0.4960174063352150
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