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

Supplementary Material

Density Functional Studies on $(NCH)_n$ AzaGraphane: Activated Surface for Organocatalysis

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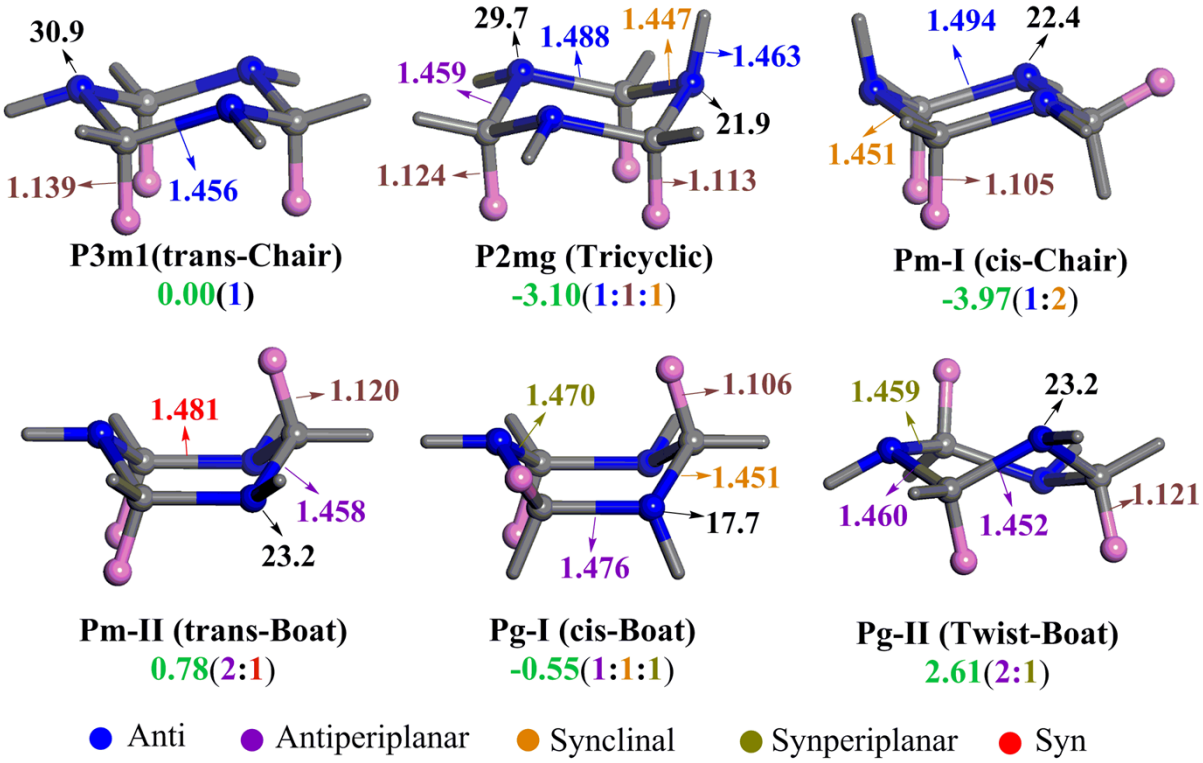
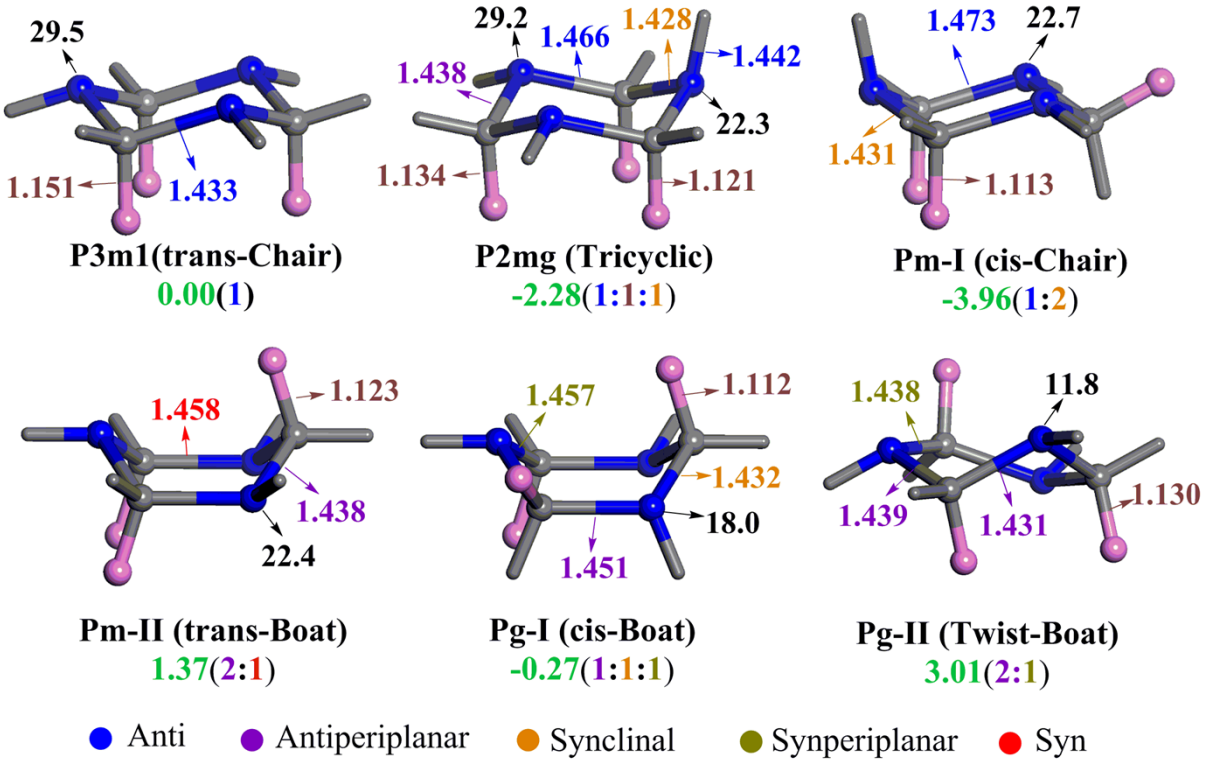
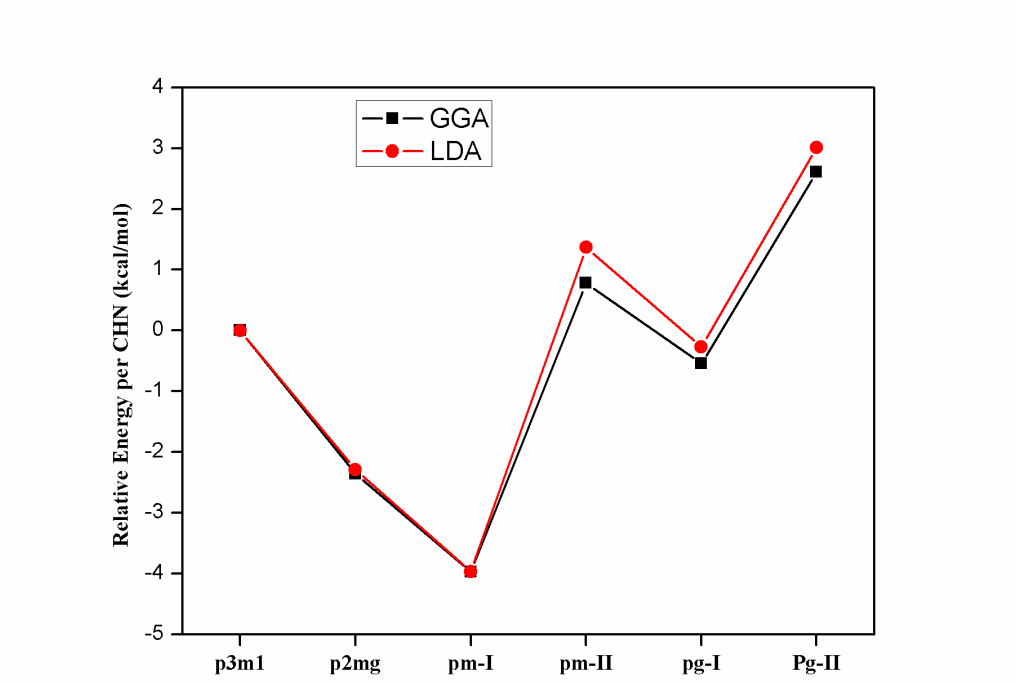
S1. Optimized geometrical parameters of (NCH)n AzaGraphanes using GGA method



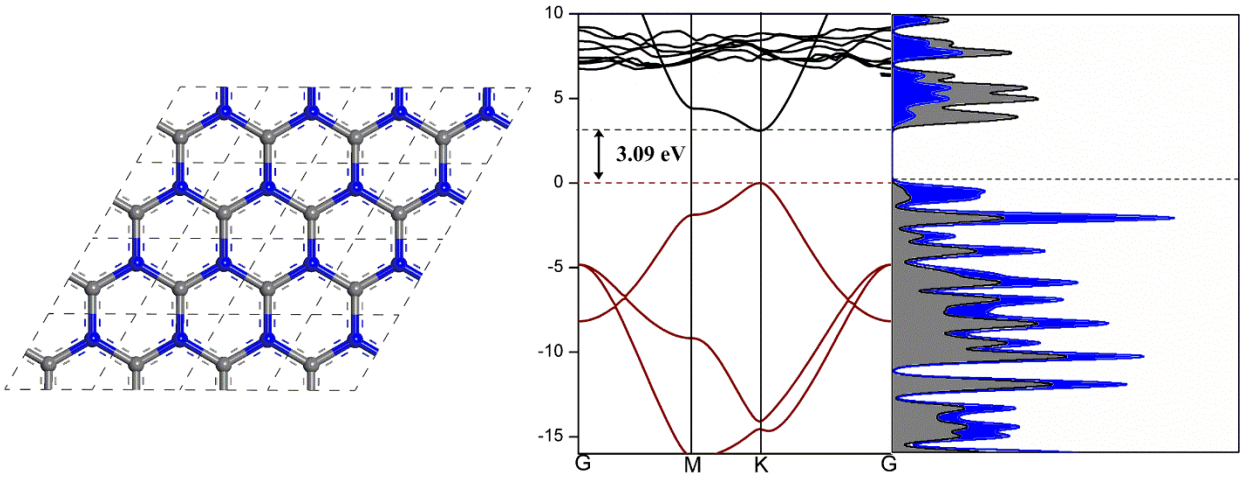
S2. Optimized geometrical parameters of (NCH)n AzaGraphanes using LDA method



S3. Comparison of relative energies for GGA and LDA method for the azagraphane isomers



S4. Band structure and PDOS of dehydrogenated Azagraphane



BN analogue of $(CN)^{+}$

S5. Total Energy, Lattice parameters and fractional coordinates of optimized (NCH)n AzaGraphanes using GGA method

1. P3m1 (Chair)

Total Energy = - 441.5475016455 eV
Lattice Parameters; a = b= 2.3808
N 0.33333 0.66667 -0.00936
C 0.66667 0.33333 0.00909
H 0.66667 0.33333 0.05295

2. P2mg (Tricyclic)

Total Energy = -1766.598628508 eV
Lattice Parameters; a= 2.3821 c = 7.2267
N -0.00000 0.06365 0.93185
C -0.00000 -0.00711 0.80334
H -0.00000 -0.06801 0.88112
C 0.50000 -0.06856 0.54511
N 0.50000 -0.00120 0.68733
H 0.50000 -0.13120 0.61265

3. Pm-I (Stirrup)

Total Energy = -883.4357836241 eV
Lattice Parameters; a = 2.3822 c= 3.5885
C -0.00000 0.02355 0.35195
H -0.00000 0.06166 0.50067
N 0.50000 0.02121 0.12183

4. Pm-II (Boat-I)

Total Energy = -883.0273714017 eV
Lattice Parameters; a = 2.3775 c = 4.0172
H -0.00000 0.05692 0.75112
C -0.00000 0.01502 0.81111
N -0.00000 0.01014 0.17839

5. Pg-I (Boat-II)

Total Energy = -1766.284607224 eV
Lattice Parameters; a =4.3409 c = 4.0027
C -0.91038 0.02172 0.55077
H -0.00300 0.05745 0.47868
N -0.39948 -0.01804 0.91701

6. Pg-II (Twist-Boat)

Total Energy = -1765.737359638 eV
Lattice Parameters; a = 4.7013 b = 4.1341
C 0.12526 0.01875 0.54061
N 0.63708 0.00745 0.86224
H 0.15329 0.06882 0.55716

S6. Total Energy, Lattice parameters and fractional coordinates of optimized (NCH)n AzaGraphanes using LDA method

1. P3m1 (Chair)

Total Energy = -442.1903507703 eV
Lattice Parameters; a = b= 2.3505
H 0.666667 0.333333 0.053061
C 0.666667 0.333333 0.008700
N 0.333333 0.666667 -0.009077

2. P2mg (Tricyclic)

Total Energy = -1769.158515355 eV
Lattice Parameters; a= 2.3528 c = 7.0817
N 0.00000 0.06441 0.93069
C 0.00000 -0.00585 0.80141
H 0.00000 -0.06747 0.88277
C 0.50000 -0.06888 0.54445
N 0.50000 -0.00108 0.68502
H 0.50000 -0.13166 0.61707

3. Pm-I (Stirrup)

Total Energy = -884.7244611970 eV
Lattice Parameters; a = 2.3548 c= 3.5141
C 0.00000 0.02353 0.34953
H 0.00000 0.06171 0.50655
N 0.50000 0.02115 0.11837

4. Pm-II (Boat-I)

Total Energy = -884.2617938318 eV
Lattice Parameters; a = 2.3478 c = 3.9614

H 0.00000 0.05706 0.74959
C 0.00000 0.01492 0.81221
N 0.00000 0.00970 0.17881

5. Pg-I (Boat-II)

Total Energy = -1768.807512688 eV
Lattice Parameters; a =4.2589 c = 3.9452
C -0.91184 0.02173 0.55225
H -0.00912 0.05751 0.47540
N -0.40007 -0.01800 0.91881

6. Pg-II (Twist-Boat)

Total Energy = -1768.239049505 eV
Lattice Parameters; a = 4.6436 b = 4.0791
C 0.12462 0.01874 0.54053
N 0.63627 0.00649 0.86297
H 0.15279 0.06916 0.55652

S7. Optimized geometrical parameters of Graphane Nanosheets using GGA method

1. P3m1 (Chair)

Total Energy = -342.2887515815 eV
Lattice Parameters; a = b= 2.5358
C 0.33333 0.66667 -0.00900
H 0.33333 0.66667 -0.05264

2. P2mg-I (Tricyclic)

Total Energy = -1369.017695313 eV
Lattice Parameters; b= 7.6856 c = 2.5385
C 0.06258 0.69363 0.25000
C -0.00179 0.55613 0.25000
H 0.11739 0.61977 0.25000
H -0.05841 0.62228 0.25000

3. Pm-I (Stirrup)

Total Energy = -684.3654977900 eV
Lattice Parameters; a = 2.5435 c= 3.8209
C 0.00000 0.02275 0.36383
H 0.00000 0.06108 0.50841

4. P2mm (Boat-I)

Total Energy = -684.1641296854 eV
Lattice Parameters; a = 2.5234 b= 4.3005
H -0.00000 0.74352 -0.05348
C -0.00000 0.81778 -0.01254

5. P2mg-II (Boat-II)

Total Energy = -1368.123494235 eV
Lattice Parameters; b = 4.5439 c = 4.3062
C 0.02111 -0.09326 -0.43181
H 0.05615 0.00993 -0.50448

6. P2gg (Twist-Boat)

Total Energy = -1367.941316739 eV
Lattice Parameters; a = 4.4097 c = 4.9755
C 0.59034 0.02135 0.61539
H 0.62177 0.09284 0.56074