Supporting Information File

Molecular Blueprints for Cleaner Air: Theoretical Insights into Cu(I)-decorated Heterocycles for Green House Gases ($CO/CO_2/CH_4$) Capture.

Abhishek Bag [a,b], Gouri Sankar Roymahapatra [b,*]

[a] *Dept. of Basic Science and Humanities, Global Institute of Science and Technology, ICARE Complex, Haldia 721657, WB, India*

[b] *School of Applied Sciences and Humanities, Haldia Institute of Technology, ICARE Complex, Haldia 721657, WB, India*
**Corresponding email: grm.chem@gmail.com; grm.chem@hithaldia.in*

Imidazole- Cu(I)@nCO_2 systems

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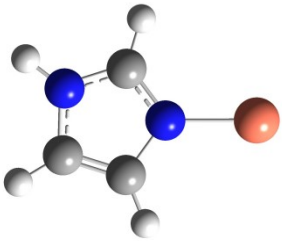
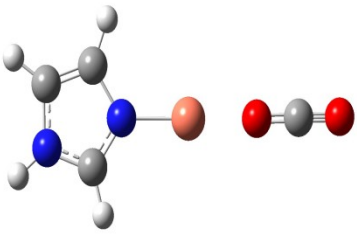
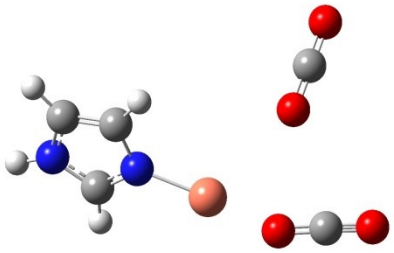
<td> 
O.E.- -50786.630 eV
Imidazole- Cu(I)</td>
<td> 
O.E.- -55919.416 eV
Imidazole- Cu(I)@1CO_2</td>
<td> 
O.E.- -61051.365 eV
Imidazole- Cu(I)@2CO_2</td>
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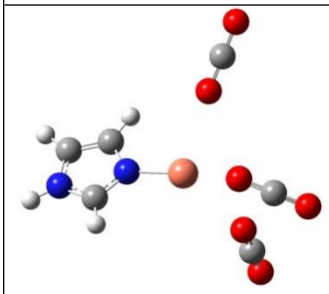
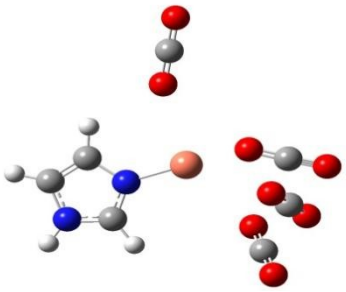
<td> 
O.E.- -66183.294 eV
Imidazole- Cu(I)@3CO_2</td>
<td> 
O.E.- -71315.219 eV
Imidazole- Cu(I)@4CO_2</td>
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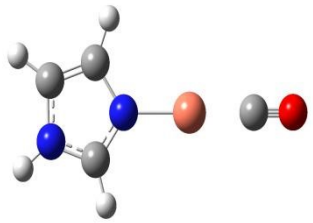
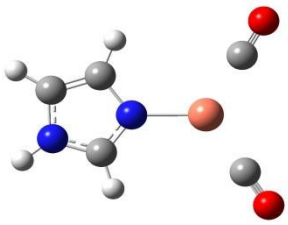
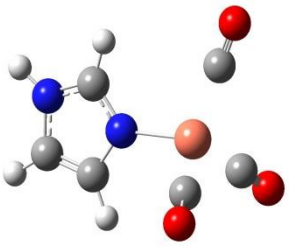
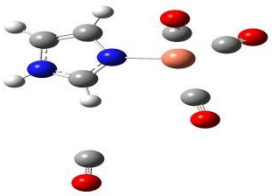
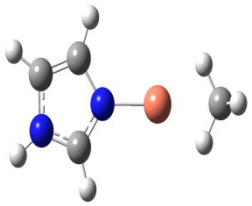
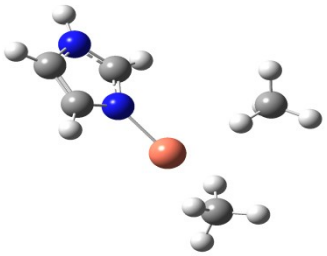
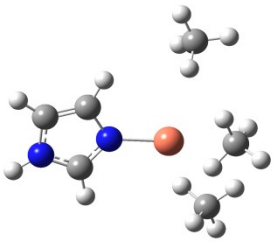
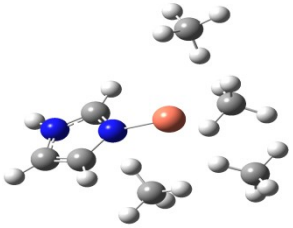
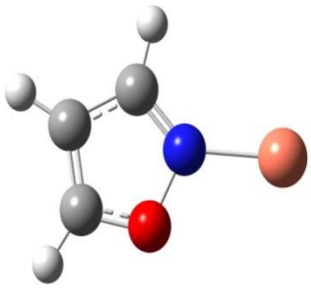
Imidazole- Cu(I)@nCO systems

 O.E.- -53871.85 eV Imidazole- Cu(I)@1CO	 O. E.- -56955.81 eV Imidazole- Cu(I)@2CO	 O.E.- -60039.74 eV Imidazole- Cu(I)@3CO
 O.E.- -63123.33 eV Imidazole- Cu(I)@4CO		

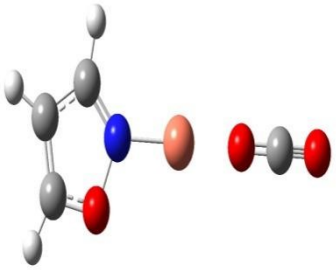
Imidazole- Cu(I)@nCH_4 systems

 O.E.- -51890.280 eV Imidazole- Cu(I)@1CH_4	 O.E.- -52993.087 eV Imidazole- Cu(I)@2CH_4	 O.E.- -54095.885 eV Imidazole- Cu(I)@3CH_4
 O.E.- -55198.687 eV Imidazole- Cu(I)@4CH_4		

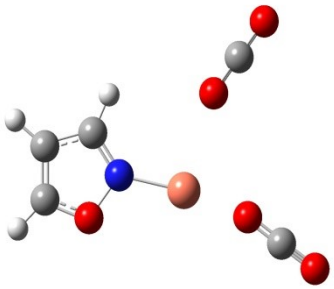
Isoxazole-Cu(I)@nCO_2 systems



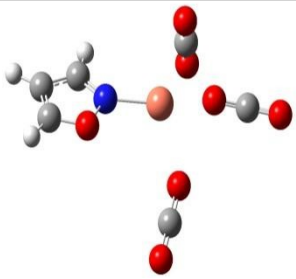
O.E.- -51325.280 eV
Isoxazole-Cu(I)



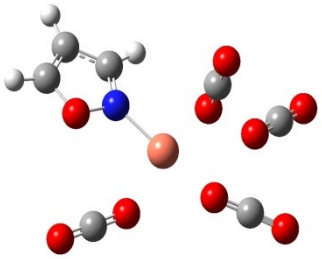
O.E.- -56458.118 eV
Isoxazole-Cu(I)@1CO_2



O.E.- -61590.090 eV
Isoxazole-Cu(I)@2CO_2

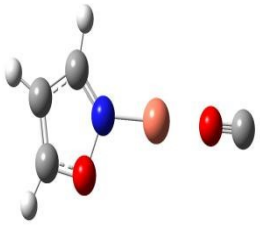


O.E.- -66722.059 eV
Isoxazole-Cu(I)@3CO_2

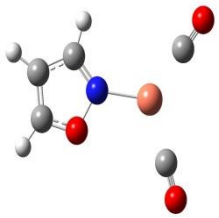


O.E.- -71853.978 eV
Isoxazole-Cu(I)@4CO_2

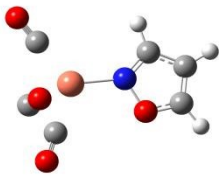
Isoxazole-Cu(I)@nCO systems



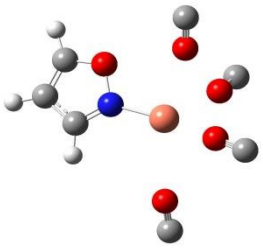
O.E.- -54409.646 eV
Isoxazole-Cu(I)@1CO



O.E.- -57494.600 eV
Isoxazole-Cu(I)@2CO

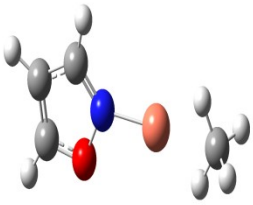


O.E.- -60578.217 eV
Isoxazole-Cu(I)@3CO

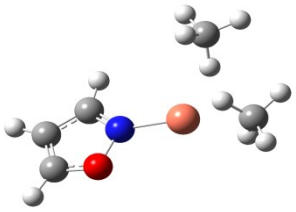


O.E.- -63660.468 eV
Isoxazole-Cu(I)@4CO

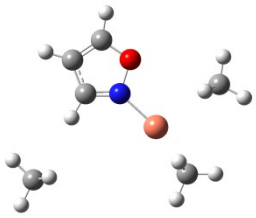
Isoxazole -Cu(I)@nCH_4 systems



O.E.- -52428.985 eV
Isoxazole -Cu(I)@1CH_4

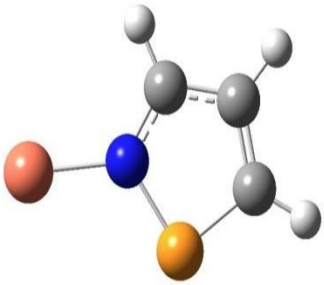


O.E.- -53531.815 eV
Isoxazole -Cu(I)@2CH_4

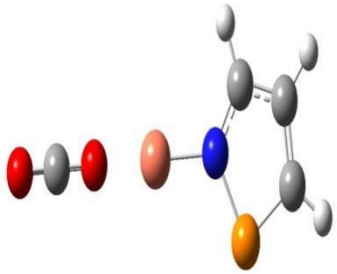


O.E.- -54634.620 eV
Isoxazole -Cu(I)@3CH_4

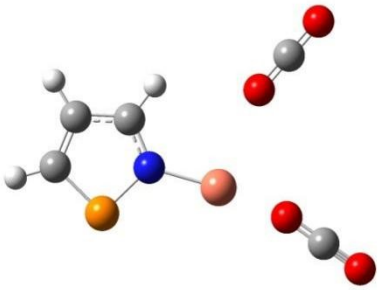
Isothiazole-Cu(I)@nCO_2 systems



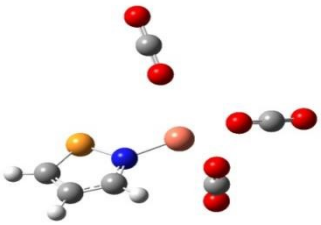
O.E.- -60114.780 eV
Isothiazole-Cu(I)



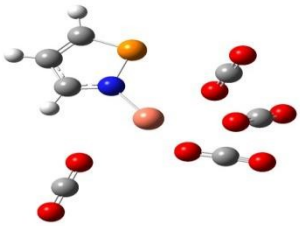
O.E.- -65247.594 eV
Isothiazole-Cu(I)@1CO_2



O.E.- -70379.559 eV
Isothiazole-Cu(I)@2CO_2

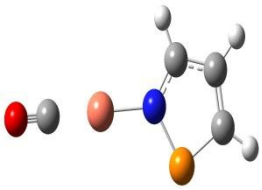


P. E.- -75511.505 eV
Isothiazole-Cu(I)@3CO_2

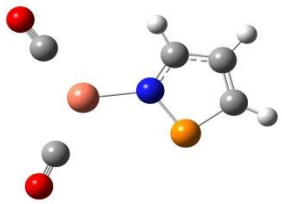


O. E.- -80643.447 eV
Isothiazole-Cu(I)@4CO_2

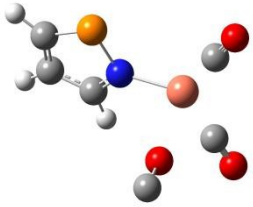
Isothiazole-Cu(I)@nCO systems



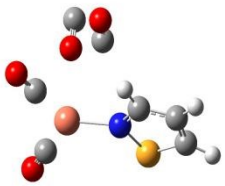
O.E.- -63200.012 eV
Isothiazole-Cu(I)@1CO



O.E.- -66284.025 eV
Isothiazole-Cu(I)@2CO

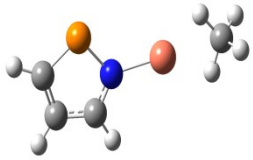


O.E.- -69367.638 eV
Isothiazole-Cu(I)@3CO

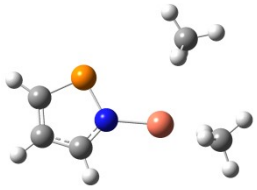


O.E.- -72451.231 eV
Isothiazole-Cu(I)@4CO

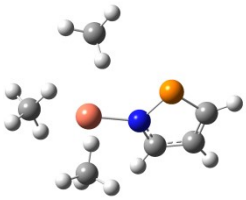
Isothiazole-Cu(I)@nCH_4 systems



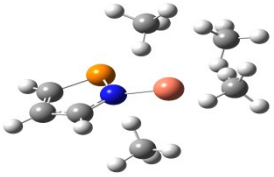
O.E.- -61218.461 eV
Isothiazole-Cu(I)@1CH_4



O.E.- -62321.280 eV
Isothiazole-Cu(I)@2CH_4

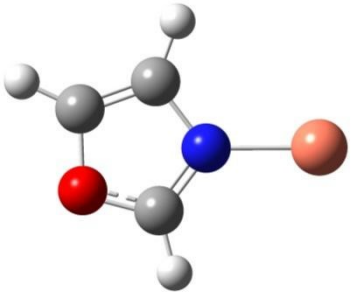


O.E.- -63424.078 eV
Isothiazole-Cu(I)@3CH_4

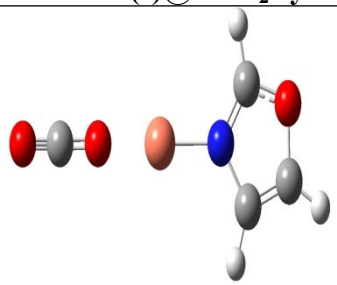


O.E.- -64526.878 eV
Isothiazole-Cu(I)@4CH_4

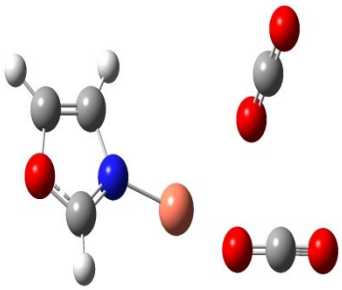
Oxazole-N-Cu(I)@nCO_2 systems



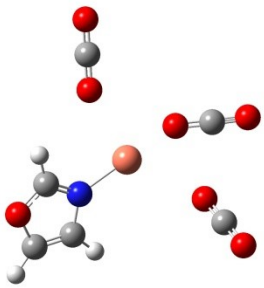
O.E.- -51326.300 eV
Oxazole-N-Cu(I)



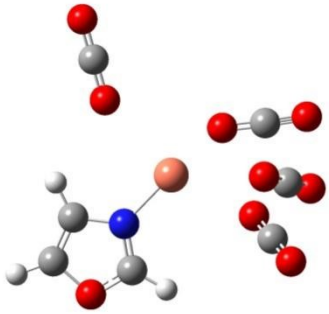
O.E.- -56459.130 eV
Oxazole-N-Cu(I)@1CO_2



O.E.- -61591.095 eV
Oxazole-N-Cu(I)@2CO_2

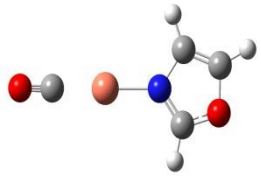


O.E.- -66723.053 eV
Oxazole-N-Cu(I)@3CO_2

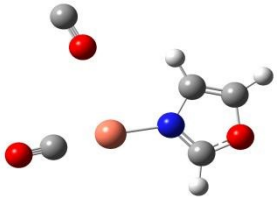


O.E.- -71854.987 eV
Oxazole-N-Cu(I)@4CO_2

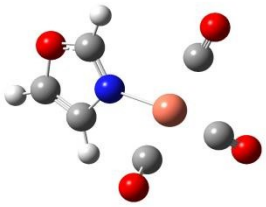
Oxazole-N-Cu(I)@nCO systems



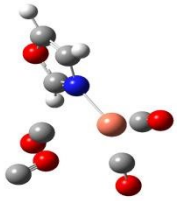
O.E.- -54411.533 eV
Oxazole-N-Cu(I)@1CO



O.E.- -57495.147 eV
Oxazole-N-Cu(I)@2CO

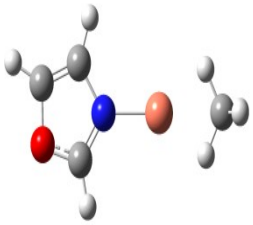


O.E.- -60579.515 eV
Oxazole-N-Cu(I)@3CO

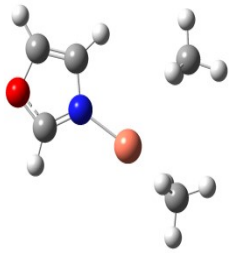


O.E.- -63662.788 eV
Oxazole-N-Cu(I)@4CO

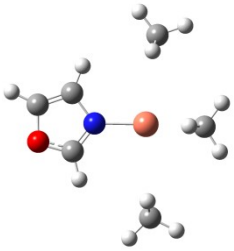
Oxazole-N-Cu(I)@nCH_4 systems



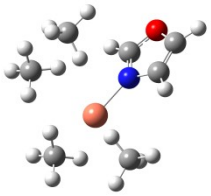
O.E.- -52429.990 eV
Oxazole-N-Cu(I)@nCH_4



O.E.- -53532.822 eV
Oxazole-N-Cu(I)@nCH_4

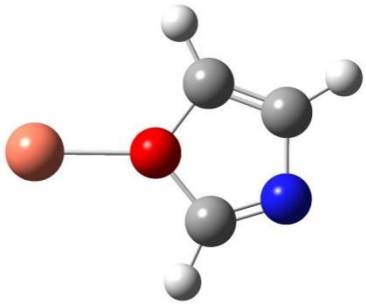


O.E.- -54635.632 eV
Oxazole-N-Cu(I)@nCH_4

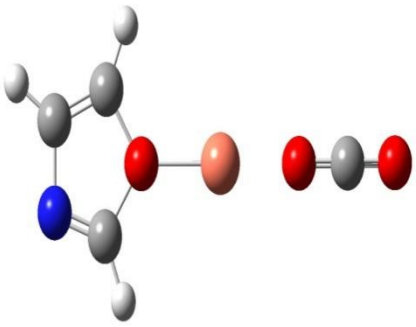


O.E.- -55738.430 eV
Oxazole-N-Cu(I)@nCH_4

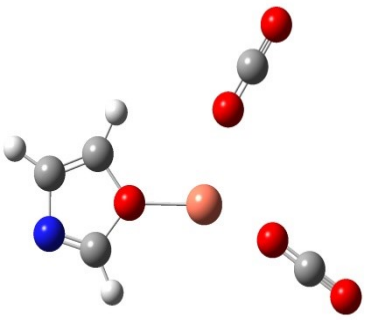
Oxazole-O-Cu(I)@nCO_2 systems



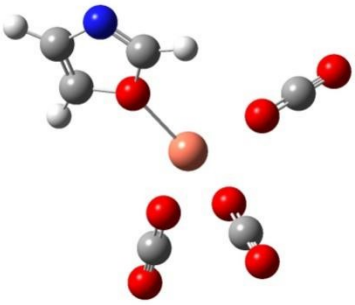
O.E.- -51324.862 eV
Oxazole-O-Cu(I)



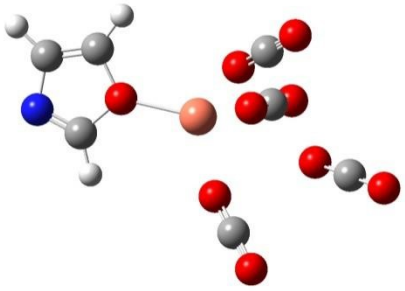
O.E.- -56457.775 eV
Oxazole-O-Cu(I)@1CO_2



O.E.- -61589.839 eV
Oxazole-O-Cu(I)@2CO_2

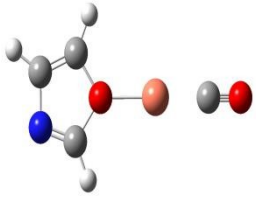


O.E.- -66721.892 eV
Oxazole-O-Cu(I)@3CO_2

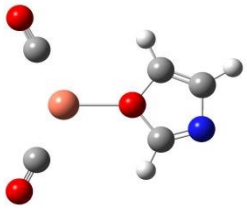


O.E.- -71853.846 eV
Oxazole-O-Cu(I)@4CO_2

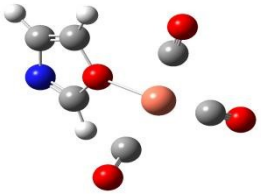
Oxazole-O-Cu(I)@nCO systems



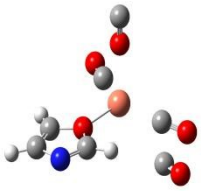
O.E.- -54410.177 eV
Oxazole-O-Cu(I)@1CO



O.E.- -57494.414 eV
Oxazole-O-Cu(I)@2CO

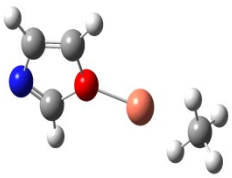


O.E.- -60578.548 eV
Oxazole-O-Cu(I)@3CO

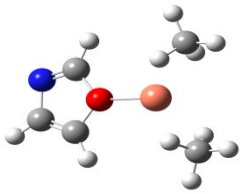


O.E.- -63661.698 eV
Oxazole-O-Cu(I)@4CO

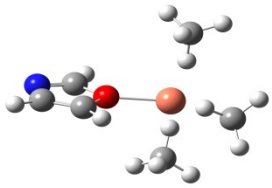
Oxazole-O-Cu(I)@nCH_4 systems



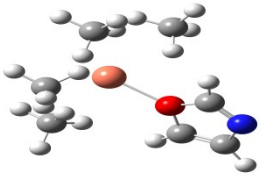
O.E.- -52428.650 eV
Oxazole-O-Cu(I)@1CH_4



O.E.- -53531.563 eV
Oxazole-O-Cu(I)@2CH_4

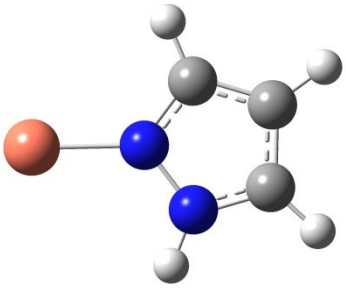


O.E.- -54634.398 eV
Oxazole-O-Cu(I)@3CH_4

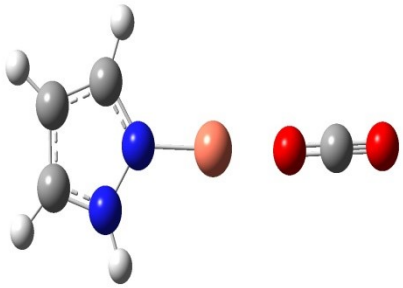


O.E.- -55737.206 eV
Oxazole-O-Cu(I)@4CH_4

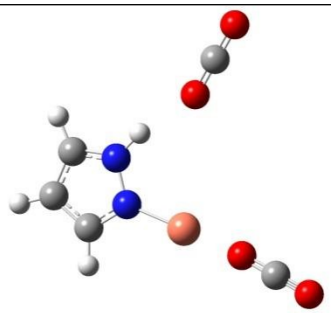
Pyrazole-Cu(I)@nCO_2 systems



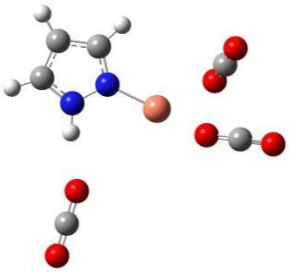
O.E.- -50785.826 eV
Pyrazole-Cu(I)



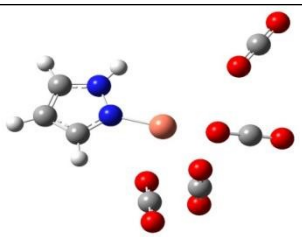
O.E.- -55918.642 eV
Pyrazole-Cu(I)@1CO_2



O.E.- -61050.659 eV
Pyrazole-Cu(I)@2CO_2

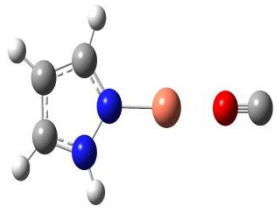
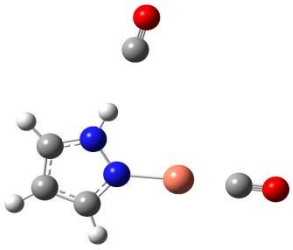
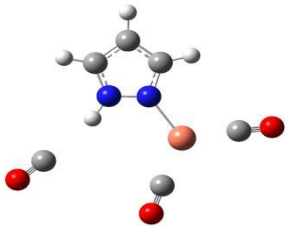


O.E.- -66182.616 eV
Pyrazole-Cu(I)@3CO_2

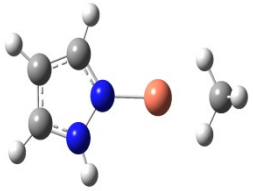
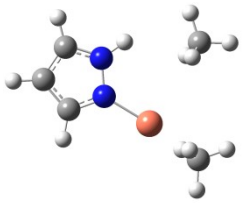
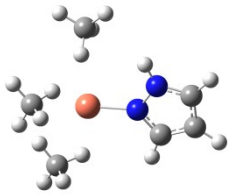
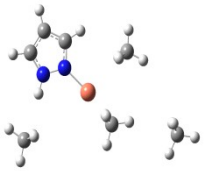


O.E.- -71314.477 eV
Pyrazole-Cu(I)@4CO_2

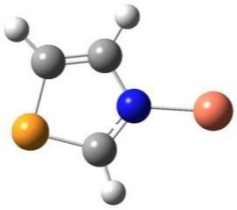
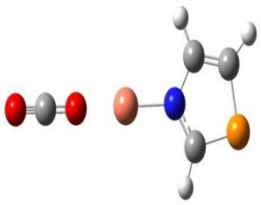
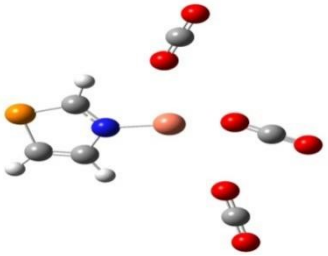
Pyrazole-Cu(I)@nCO systems

 O.E.- -53870.179 eV Pyrazole-Cu(I)@1CO	 O.E.- -56954.774 eV Pyrazole-Cu(I)@2CO	 O.E.- -60038.760 eV Pyrazole-Cu(I)@3CO

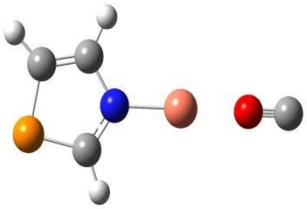
Pyrazole-Cu(I)@nCH4 systems

 O.E.- -51889.506 eV Pyrazole-Cu(I)@1CH_4	 O.E.- -52992.347 eV Pyrazole-Cu(I)@2CH_4	 O.E.- -54095.147 eV Pyrazole-Cu(I)@3CH_4
 O.E.- -55197.955 eV Pyrazole-Cu(I)@4CH_4		

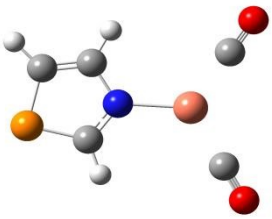
Thiazole-Cu(I)@nCO_2 systems

 O.E.- -60115.003 eV Thiazole-Cu(I)	 O.E.- -65247.807 eV Thiazole-Cu(I)@1CO_2	 O.E.- -70379.758 eV Thiazole-Cu(I)@2CO_2
 O.E.- -75511.714 eV Thiazole-Cu(I)@3CO_2		

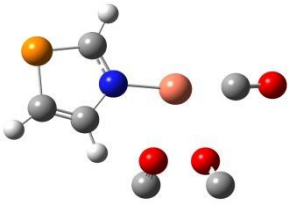
Thiazole-Cu(I)@nCO systems



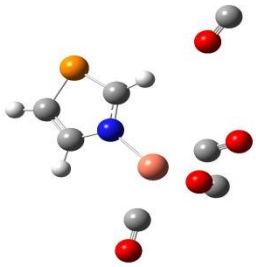
O.E.- -63199.345 eV
Thiazole-Cu(I)@1CO



O.E.- -66284.212 eV
Thiazole-Cu(I)@2CO

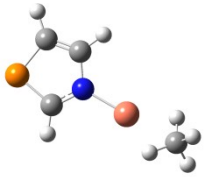


O.E.- -69367.426 eV
Thiazole-Cu(I)@3CO

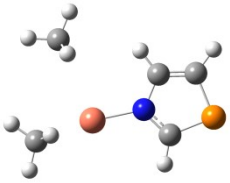


O.E.- -72451.409 eV
Thiazole-Cu(I)@4CO

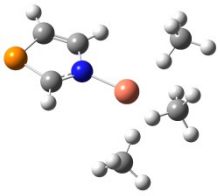
Thiazole-Cu(I)@nCH$_4$ systems



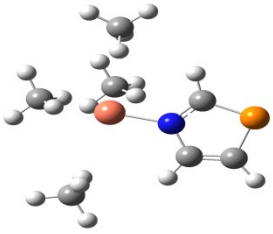
O.E.- -61218.668 eV
Thiazole-Cu(I)@1CH$_4$



O.E.- -62321.491 eV
Thiazole-Cu(I)@2CH$_4$



O.E.- -63424.290 eV
Thiazole-Cu(I)@3CH$_4$



O.E.- -64527.097 eV
Thiazole-Cu(I)@4CH$_4$

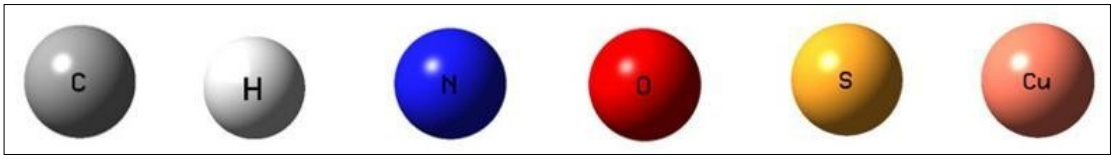


Fig. SF1: *Optimized geometries and energy of Cu(I) decorated and gradual GHGs adsorb different aromatic five-membered heterocyclic systems decorated with Cu(I) at B3LYP/6–31+g (d, p) level of theory.*

Table ST1: *Electrophilicity (ω) and (eV),Hardness (η); (eV) of gradual GHGs adsorb different model systems decorated with Cu(I) at B3LYP/6–31+g (d, p) level of theory.*

Imidazole system

System	Electrophilicity	System	Electrophilicity	System	Electrophilicity
Imidazole-Cu	11.224	**Imidazole-Cu**	11.224	**Imidazole-Cu**	11.224
Imidazole-Cu@1CO	8.489	**Imidazole-Cu@1CO_2**	5.594	**Imidazole-Cu@1CH_4**	5.068
Imidazole-Cu@2CO	9.142	**Imidazole-Cu@2CO_2**	5.259	**Imidazole-Cu@2CH_4**	4.834
Imidazole-Cu@3CO	7.561	**Imidazole-Cu@3CO_2**	4.977	**Imidazole-Cu@ 3CH_4**	4.716
Imidazole-Cu@ 4CO	7.489	**Imidazole-Cu@ 4CO_2**	4.771	**Imidazole-Cu@ 4CH_4**	4.576

Isoxazole System

System	Electrophilicity	System	Electrophilicity	System	Electrophilicity
Isoxazole-Cu	11.137	**Isoxazole-Cu**	11.137	**Isoxazole-Cu**	11.137
Isoxazole-Cu@1CO	7.103	**Isoxazole-Cu@1CO_2**	6.351	**Isoxazole-Cu@ 1CH_4**	6.399
Isoxazole-Cu@2CO	8.759	**Isoxazole-Cu@2CO_2**	6.070	**Isoxazole-Cu@ 2CH_4**	6.214
Isoxazole-Cu@3CO	8.141	**Isoxazole-Cu@3CO_2**	6.047	**Isoxazole-Cu@ 3CH_4**	6.104
Isoxazole-Cu@ 4CO	6.495	**isoxazoleCu4CO_2**	5.997		

Isothiazole System

System	Electrophilicity	System	Electrophilicity	System	Electrophilicity
Isothiazole-Cu	11.260	**Isothiazole-Cu**	11.260	**Isothiazole-Cu**	11.260
Isothiazole-Cu@1CO	8.437	**Isothiazole-Cu@1CO_2**	6.720	**Isothiazole-Cu@1CH_4**	6.779
Isothiazole-Cu@2CO	8.992	**Isothiazole-Cu2@CO_2**	6.421	**Isothiazole-Cu@2CH_4**	6.595
Isothiazole-Cu@3CO	8.354	**Isothiazole-Cu@3CO_2**	6.431	**Isothiazole-Cu@3CH_4**	6.500
Isothiazole-Cu@4CO	8.290	**Isothiazole-Cu4@CO_2**	6.299	**Isothiazole-Cu@4CH_4**	6.422

Pyrazole System

System	Electrophilicity	System	Electrophilicity	System	Electrophilicity
Pyrazole-Cu	11.655	**Pyrazole-Cu**	11.655	**Pyrazole-Cu**	11.655
Pyrazole-Cu@1CO	7.216	**Pyrazole-Cu@1CO_2**	5.888	**Pyrazole-Cu@1CH_4**	5.400
Pyrazole-Cu@2CO	8.628	**Pyrazole-Cu@2CO_2**	5.673	**Pyrazole-Cu@2CH_4**	5.083
Pyrazole-Cu@3CO	9.179	**Pyrazole-Cu@3CO_2**	5.344	**Pyrazole-Cu@3CH_4**	4.940
Pyrazole-Cu@4CO	----------	**Pyrazole-Cu@4CO_2**	4.993	**Pyrazole-Cu@4CH_4**	4.919

Thiazole System

System	Electrophilicity	System	Electrophilicity	System	Electrophilicity
Thiazole-Cu	11.655	**Thiazole-Cu**	11.421	**Thiazole-Cu**	11.421
Thiazole-Cu@1CO	7.163	**Thiazole-Cu@1CO_2**	6.231	**Thiazole-Cu@1CH_4**	6.289
Thiazole-Cu@2CO	9.281	**Thiazole-Cu@2CO_2**	5.996	**Thiazole-Cu@2CH_4**	6.127
Thiazole-Cu@3CO	7.819	**Thiazole-Cu@3CO_2**	5.815	**Thiazole-Cu@3CH_4**	6.033
Thiazole-Cu@4CO	8.508	**Thiazole-Cu@4CO_2**	--------	**Thiazole-Cu@4CH_4**	5.968

Oxazole-O System

System	Electrophilicity	System	Electrophilicity	System	Electrophilicity
Oxazole-O-Cu	17.036	**Oxazole-O-Cu**	17.036	**Oxazole-O-Cu**	17.036
Oxazole-O-Cu @1CO	10.254	**Oxazole-O-Cu @1CO_2**	7.738	**Oxazole-O-Cu @1CH_4**	7.284
Oxazole-O-Cu @2CO	11.545	**Oxazole-O-Cu @2CO_2**	6.876	**Oxazole-O-Cu @2CH_4**	6.470
Oxazole-O-Cu @3CO	10.835	**Oxazole-O-Cu @3CO_2**	6.051	**Oxazole-O-Cu @3CH_4**	6.141
Oxazole-O-Cu @4 CO	10.162	**Oxazole-O-Cu @ 4 CO_2**	5.864	**Oxazole-O-Cu @4CH_4**	5.910

Oxazole-N System

System	Electrophilicity	System	Electrophilicity	System	Electrophilicity
Oxazole-N-Cu	11.640	**Oxazole-N-Cu**	11.640	**Oxazole-N-Cu**	11.640
Oxazole-N-Cu@1CO	8.697	**Oxazole-N-Cu@1CO_2**	5.911	**Oxazole-N-Cu @1CH_4**	5.677
Oxazole-N-Cu@2CO	8.353	**Oxazole-N-Cu@2CO_2**	5.536	**Oxazole-N-Cu @2CH_4**	5.500
Oxazole-N-Cu@3CO	7.840	**Oxazole-N-Cu@3CO_2**	5.304	**Oxazole-N-Cu @3CH_4**	5.408
Oxazole-N-Cu@4CO	8.557	**Oxazole-N-Cu@4CO_2**	5.147	**Oxazole-N-Cu @4CH_4**	5.319

Imidazole system

System	Hardness	System	Hardness	System	Hardness
Imidazole-Cu	3.949	**Imidazole-Cu**	3.949	**Imidazole-Cu**	3.949
Imidazole-Cu@1CO	4.699	**Imidazole-Cu@1CO_2**	5.870	**Imidazole-Cu@1CH_4**	6.248
Imidazole-Cu@2CO	4.308	**Imidazole-Cu@2CO_2**	6.003	**Imidazole-Cu@2CH_4**	6.333
Imidazole-Cu@3CO	4.729	**Imidazole-Cu@3CO_2**	6.057	**Imidazole-Cu@ 3CH_4**	6.386
Imidazole-Cu@4CO	4.684	**Imidazole-Cu@4CO_2**	6.128	**Imidazole-Cu@ 4CH_4**	6.443

Isoxazole System

System	Hardness	System	Hardness	System	Hardness
Isoxazole-Cu	4.579	**Isoxazole-Cu**	4.579	**Isoxazole-Cu**	4.579
Isoxazole-Cu@1CO	5.936	**Isoxazole-Cu@1CO_2**	6.167	**Isoxazole-Cu@ 1CH_4**	6.235
Isoxazole-Cu@2CO	5.166	**Isoxazole-Cu@2CO_2**	6.002	**Isoxazole-Cu@ 2CH_4**	6.161
Isoxazole-Cu@3CO	5.340	**Isoxazole-Cu@3CO_2**	5.658	**Isoxazole-Cu@ 3CH_4**	6.165
Isoxazole-Cu@4CO	5.800	**Isoxazole-Cu@4CO_2**	5.584		

Isothiazole System

System	Hardness	System	Hardness	System	Hardness
Isothiazole-Cu	4.332	**Isothiazole-Cu**	4.332	**Isothiazole-Cu**	4.332
Isothiazole-Cu@1CO	5.189	**Isothiazole-Cu@1CO_2**	5.758	**Isothiazole-Cu@1CH_4**	5.778
Isothiazole-Cu@2CO	4.811	**Isothiazole-Cu2@CO_2**	5.726	**Isothiazole-Cu@2CH_4**	5.763
Isothiazole-Cu@3CO	4.990	**Isothiazole-Cu@3CO_2**	5.501	**Isothiazole-Cu@3CH_4**	5.781
Isothiazole-Cu@4CO	4.950	**Isothiazole-Cu4@CO_2**	5.446	**Isothiazole-Cu@4CH_4**	5.781

Pyrazole System

System	Hardness	System	Hardness	System	Hardness
Pyrazole-Cu	4.086	**Pyrazole-Cu**	4.086	**Pyrazole-Cu**	4.086
Pyrazole-Cu@1CO	5.437	**Pyrazole-Cu@1CO_2**	6.000	**Pyrazole-Cu@1CH_4**	6.373
Pyrazole-Cu@2CO	4.831	**Pyrazole-Cu@2CO_2**	5.938	**Pyrazole-Cu@2CH_4**	6.456
Pyrazole-Cu@3CO	4.487	**Pyrazole-Cu@3CO_2**	6.040	**Pyrazole-Cu@3CH_4**	6.511
Pyrazole-Cu@4CO	----------	**Pyrazole-Cu@4CO_2**	6.198	**Pyrazole-Cu@4CH_4**	6.464

Thiazole System

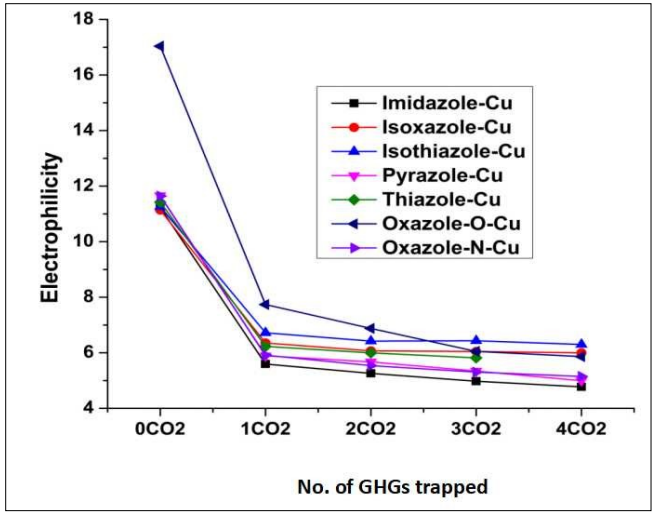
System	Hardness	System	Hardness	System	Hardness
Thiazole-Cu	4.086	**Thiazole-Cu**	4.169	**Thiazole-Cu**	4.169
Thiazole-Cu@1CO	5.499	**Thiazole-Cu@1CO_2**	5.878	**Thiazole-Cu@1CH_4**	5.876
Thiazole-Cu@2CO	4.551	**Thiazole-Cu@2CO_2**	5.902	**Thiazole-Cu@2CH_4**	5.879
Thiazole-Cu@3CO	5.148	**Thiazole-Cu@3CO_2**	5.879	**Thiazole-Cu@3CH_4**	5.889
Thiazole-Cu@4CO	4.713	**Thiazole-Cu@4CO_2**	--------	**Thiazole-Cu@4CH_4**	5.888

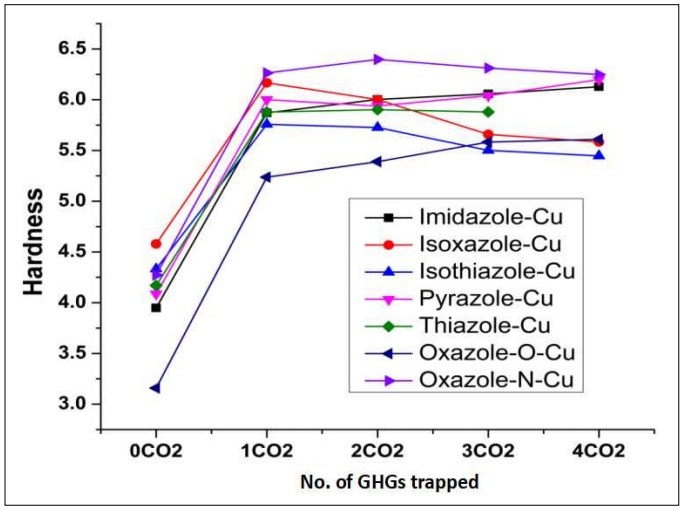
Oxazole-O System

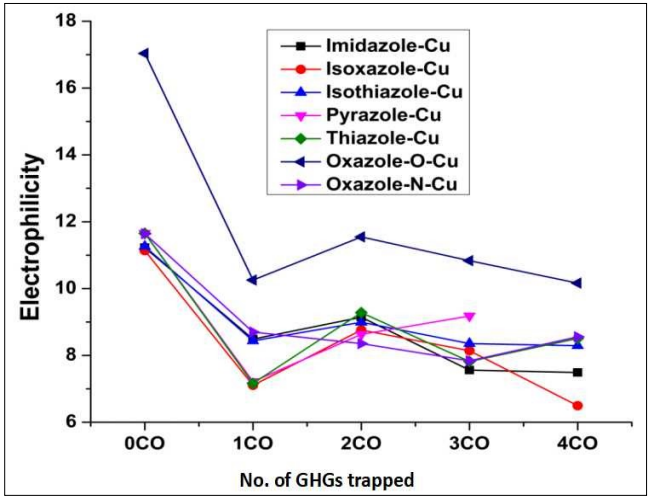
System	Hardness	System	Hardness	System	Hardness
Oxazole-O-Cu	3.159	**Oxazole-O-Cu**	3.159	**Oxazole-O-Cu**	3.159
Oxazole-O-Cu@1CO	4.493	**Oxazole-O-Cu@1CO_2**	5.237	**Oxazole-O-Cu@1CH_4**	5.461
Oxazole-O-Cu@2CO	3.894	**Oxazole-O-Cu@2CO_2**	5.390	**Oxazole-O-Cu@2CH_4**	5.582
Oxazole-O-Cu@3CO	3.880	**Oxazole-O-Cu@3CO_2**	5.583	**Oxazole-O-Cu@3CH_4**	5.682
Oxazole-O-Cu@4CO	4.113	**Oxazole-O-Cu@4CO_2**	5.609	**Oxazole-O-Cu@4CH_4**	5.787

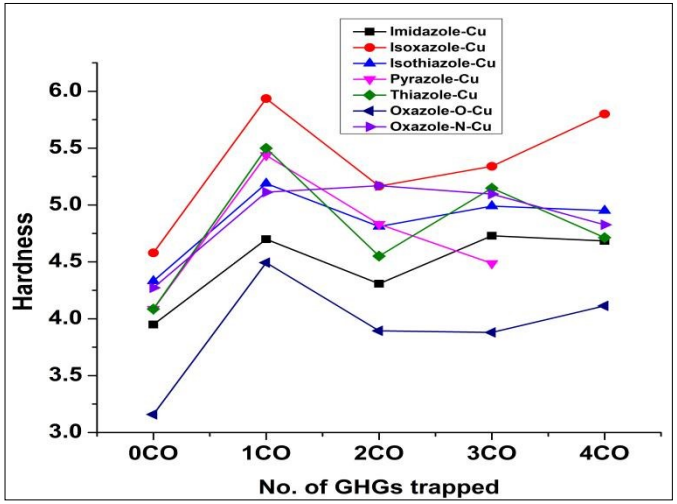
Oxazole-N System

System	Hardness	System	Hardness	System	Hardness
Oxazole-O-Cu	4.272	**Oxazole-N-Cu**	4.272	**Oxazole-N-Cu**	4.272
Oxazole-O-Cu@1CO	5.113	**Oxazole-N-Cu@1CO_2**	6.264	**Oxazole-N-Cu@1CH_4**	6.454
Oxazole-O-Cu@2CO	5.170	**Oxazole-N-Cu@2CO_2**	6.397	**Oxazole-N-Cu@2CH_4**	6.455
Oxazole-O-Cu@3CO	5.096	**Oxazole-N-Cu@3CO_2**	6.312	**Oxazole-N-Cu@3CH_4**	6.456
Oxazole-O-Cu@4CO	4.826	**Oxazole-N-Cu@4CO_2**	6.249	**Oxazole-N-Cu@4CH_4**	6.475


Electrophilicity
No. of GHGs trapped
0CO2
1CO2
2CO2
3CO2
4CO2
Imidazole-Cu
Isoxazole-Cu
Isothiazole-Cu
Pyrazole-Cu
Thiazole-Cu
Oxazole-O-Cu
Oxazole-N-Cu


Hardness
No. of GHGs trapped
0CO2
1CO2
2CO2
3CO2
4CO2
Imidazole-Cu
Isoxazole-Cu
Isothiazole-Cu
Pyrazole-Cu
Thiazole-Cu
Oxazole-O-Cu
Oxazole-N-Cu


Electrophilicity
No. of GHGs trapped
0CO
1CO
2CO
3CO
4CO
Imidazole-Cu
Isoxazole-Cu
Isothiazole-Cu
Pyrazole-Cu
Thiazole-Cu
Oxazole-O-Cu
Oxazole-N-Cu


Hardness
No. of GHGs trapped
0CO
1CO
2CO
3CO
4CO
Imidazole-Cu
Isoxazole-Cu
Isothiazole-Cu
Pyrazole-Cu
Thiazole-Cu
Oxazole-O-Cu
Oxazole-N-Cu

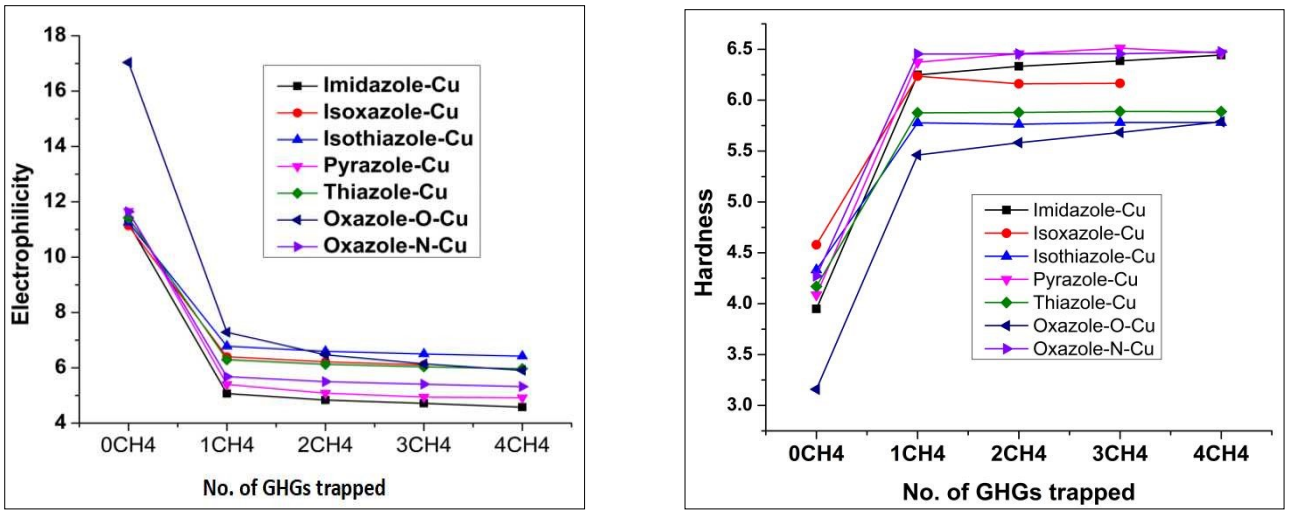


Fig. SF2: *Graphical reprasentation of Electrophilicity (ω) and (eV),Hardness (η); (eV) of gradual GHGs adsorbed different aromatic five-membered heterocyclic systems decorated with Cu(I) at B3LYP/6–31+g (d, p) level of theory.*

Table ST2: *Average Adsorption energy values of gradual GHGs adsorb different model systems decorated with Cu(I) at B3LYP/6–31+g (d, p) level of theory.*

Imidazole system

System	Adv. Adsorption Energy	System	Adv. Adsorption Energy	System	Adv. Adsorption Energy
Imidazole-Cu@1CO	1.698	**Imidazole-Cu@1CO_2**	0.977	**Imidazole-Cu@1CH_4**	0.876
Imidazole-Cu@2CO	1.071	**Imidazole-Cu@2CO_2**	0.559	**Imidazole-Cu@2CH_4**	0.455
Imidazole-Cu@3CO	0.848	**Imidazole-Cu@3CO_2**	0.413	**Imidazole-Cu@3CH_4**	0.312

Imidazole-Cu@4CO	0.654	**Imidazole-Cu@4CO_2**	0.339	**Imidazole-Cu@4CH_4**	0.241

.

System	Adv. Adsorption Energy	System	Adv. Adsorption Energy	System	Adv. Adsorption Energy
Isoxazole-Cu@1CO	0.842	**Isoxazole-Cu@1CO_2**	1.028	**Isoxazole-Cu@1CH_4**	0.931
Isoxazole-Cu@2CO	1.137	**Isoxazole-Cu@2CO_2**	0.596	**Isoxazole-Cu@2CH_4**	0.494
Isoxazole-Cu@3CO	0.790	**Isoxazole-Cu@3CO_2**	0.451	**Isoxazole-Cu@3CH_4**	0.340
Isoxazole-Cu@4CO	0.274	**Isoxazole-Cu@4CO_2**	0.366		

Isothiazole System

System	Adv. Adsorption Energy	System	Adv. Adsorption Energy	System	Adv. Adsorption Energy
Isothiazole-Cu@1CO	1.708	**Isothiazole-Cu@1CO_2**	1.006	**Isothiazole-Cu@1CH_4**	0.906
Isothiazole-Cu@2CO	1.099	**Isothiazole-Cu2@CO_2**	0.581	**Isothiazole-Cu@2CH_4**	0.476
Isothiazole-Cu@3CO	0.763	**Isothiazole-Cu@3CO_2**	0.433	**Isothiazole-Cu@3CH_4**	0.326
Isothiazole-Cu@4CO	0.590	**Isothiazole-Cu4@CO_2**	0.359	**Isothiazole-Cu@4CH_4**	0.251

Pyrazole System

System	Adv. Adsorption Energy	System	Adv. Adsorption Energy	System	Adv. Adsorption Energy
Pyrazole-Cu@1CO	0.831	**Pyrazole-Cu@1CO_2**	0.819	**Pyrazole-Cu@1CH_4**	0.907

Pyrazole-Cu@2CO	0.951	**Pyrazole-Cu@2CO_2**	1.082	**Pyrazole-Cu@2CH_4**	0.487
Pyrazole-Cu@3CO	0.788	**Pyrazole-Cu@3CO_2**	0.618	**Pyrazole-Cu@3CH_4**	0.334
Pyrazole-Cu@4CO	----------	**Pyrazole-Cu@4CO_2**	0.579	**Pyrazole-Cu@4CH_4**	0.259

Thiazole System

System	Adv. Adsorption Energy	System	Adv. Adsorption Energy	System	Adv. Adsorption Energy
Thiazole-Cu@1CO	0.819	**Thiazole-Cu@1CO_2**	0.996	**Thiazole-Cu@1CH_4**	0.892
Thiazole-Cu@2CO	1.082	**Thiazole-Cu@2CO_2**	0.569	**Thiazole-Cu@2CH_4**	0.471
Thiazole-Cu@3CO	0.618	**Thiazole-Cu@3CO_2**	0.429	**Thiazole-Cu@3CH_4**	0.322
Thiazole-Cu@4CO	0.579	**Thiazole-Cu@4CO_2**	--------	**Thiazole-Cu@4CH_4**	0.250

Oxazole-O System

System	Adv. Adsorption Energy	System	Adv. Adsorption Energy	System	Adv. Adsorption Energy
Oxazole-O-Cu@1CO	1.793	**Oxazole-O-Cu@1CO_2**	1.104	**Oxazole-O-Cu@1CH_4**	1.015
Oxazole-O-Cu@2CO	1.253	**Oxazole-O-Cu@2CO_2**	0.680	**Oxazole-O-Cu@2CH_4**	0.577
Oxazole-O-Cu@3CO	1.039	**Oxazole-O-Cu@3CO_2**	0.535	**Oxazole-O-Cu@3CH_4**	0.405
Oxazole-O-Cu@4CO	0.686	**Oxazole-O-Cu@4CO_2**	0.438	**Oxazole-O-Cu@4CH_4**	0.313

Oxazole-N System

System	Adv. Adsorption Energy	System	Adv. Adsorption Energy	System	Adv. Adsorption Energy
Oxazole-O-Cu@1CO	1.711	**Oxazole-N-Cu@1CO_2**	1.023	**Oxazole-N-Cu @1CH_4**	0.918
Oxazole-O-Cu@2CO	0.901	**Oxazole-N-Cu@2CO_2**	0.590	**Oxazole-N-Cu @2CH_4**	0.488

Oxazole-O-Cu@3CO	0.882	**Oxazole-N-Cu@3CO_2**	0.443	**Oxazole-N-Cu @3CH_4**	0.338
Oxazole-O-Cu@4CO	0.599	**Oxazole-N-Cu@4CO_2**	0.364	**Oxazole-N-Cu @4CH_4**	0.259

Table ST3: NBO charges on metal center of gradual green house gases adsorb different aromatic model systems decorated with Cu(I) at B3LYP/6–31+g (d, p) level of theory.

Imidazole system

System	NBO	System	NBO	System	NBO
Imidazole-Cu	0.863	**Imidazole-Cu**	0.863	**Imidazole-Cu**	0.863
Imidazole-Cu@1CO	0.626	**Imidazole-Cu@1CO_2**	0.759	**Imidazole-Cu@1CH_4**	0.737
Imidazole-Cu@2CO	0.372	**Imidazole-Cu@2CO_2**	0.754	**Imidazole-Cu@2CH_4**	0.731
Imidazole-Cu@3CO	-0.029	**Imidazole-Cu@3CO_2**	0.744	**Imidazole-Cu@3CH_4**	0.733
Imidazole-Cu@4CO	-0.029	**Imidazole-Cu@4CO_2**	0.742	**Imidazole-Cu@4CH_4**	0.730

Isoxazole System

System	NBO	System	NBO	System	NBO
Isoxazole-Cu	0.890	**Isoxazole-Cu**	0.89	**Isoxazole-Cu**	0.890
Isoxazole-Cu@1CO	0.788	**Isoxazole-Cu@1CO_2**	0.781	**Isoxazole-Cu@ 1CH_4**	0.752
Isoxazole-Cu@2CO	0.376	**Isoxazole-Cu@2CO_2**	0.771	**Isoxazole-Cu@ 2CH_4**	0.736
Isoxazole-Cu@3CO	0.351	**Isoxazole-Cu@3CO_2**	0.742	**Isoxazole-Cu@ 3CH_4**	0.727

Isoxazole-Cu@ 4CO	0.735	**isoxazoleCu4CO_2**	0.741

Isothiazole System

System	NBO	System	NBO	System	NBO
Isothiazole-Cu	0.877	**Isothiazole-Cu**	0.877	**Isothiazole-Cu**	0.877
Isothiazole-Cu@1CO	0.634	**Isothiazole-Cu@1CO_2**	0.774	**Isothiazole-Cu@1CH_4**	0.746
Isothiazole-Cu@2CO	0.377	**Isothiazole-Cu2@CO_2**	0.764	**Isothiazole-Cu@2CH_4**	0.732
Isothiazole-Cu@3CO	0.353	**Isothiazole-Cu@3CO_2**	0.751	**Isothiazole-Cu@3CH_4**	0.727
Isothiazole-Cu@4CO	0.354	**Isothiazole-Cu4@CO_2**	0.737	**Isothiazole-Cu@4CH_4**	0.721

Pyrazole System

System	NBO	System	NBO	System	NBO
Pyrazole-Cu	0.861	**Pyrazole-Cu**	0.861	**Pyrazole-Cu**	0.861
Pyrazole-Cu@1CO	0.763	**Pyrazole-Cu@1CO_2**	0.755	**Pyrazole-Cu@1CH_4**	0.729
Pyrazole-Cu@2CO	0.613	**Pyrazole-Cu@2CO_2**	0.754	**Pyrazole-Cu@2CH_4**	0.727

Pyrazole-Cu@3CO	0.358	**Pyrazole-Cu@3CO_2**	0.748	**Pyrazole-Cu@3CH_4**	0.728
Pyrazole-Cu@4CO	----------	**Pyrazole-Cu@4CO_2**	0.732	**Pyrazole-Cu@4CH_4**	0.721

Thiazole System

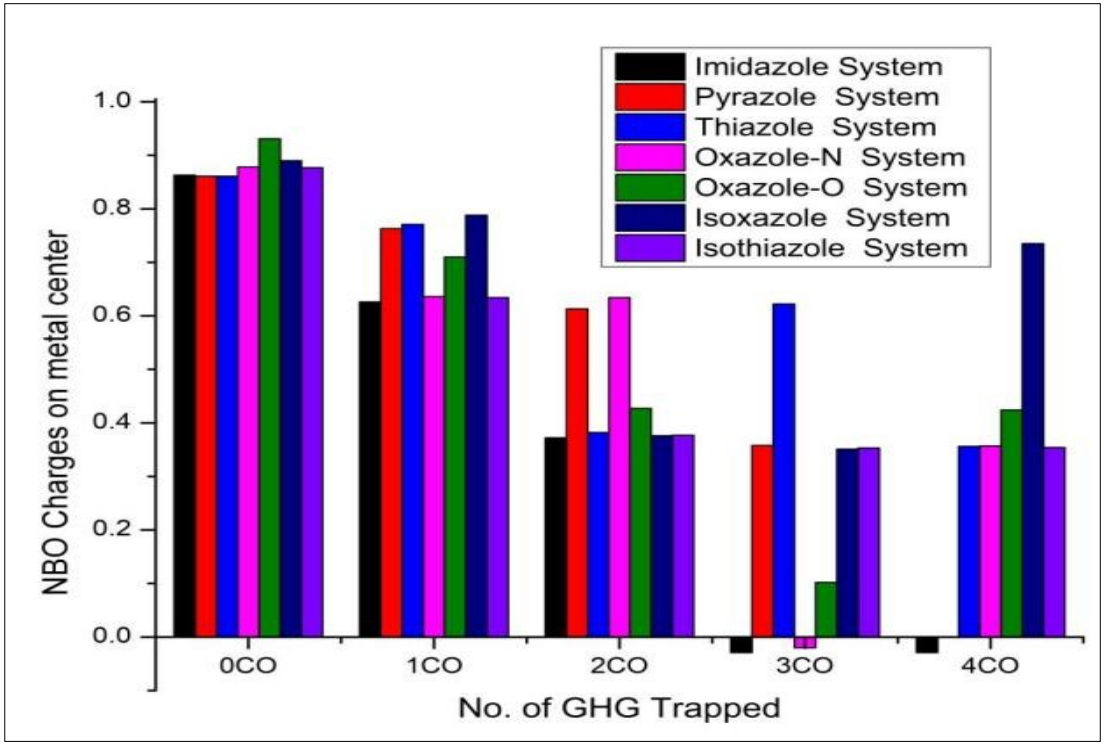
System	NBO	System	NBO	System	NBO
Thiazole-Cu	0.861	**Thiazole-Cu**	0.861	**Thiazole-Cu**	0.861
Thiazole-Cu@1CO	0.771	**Thiazole-Cu@1CO_2**	0.765	**Thiazole-Cu@1CH_4**	0.743
Thiazole-Cu@2CO	0.382	**Thiazole-Cu@2CO_2**	0.761	**Thiazole-Cu@2CH_4**	0.735
Thiazole-Cu@3CO	0.622	**Thiazole-Cu@3CO_2**	0.752	**Thiazole-Cu@3CH_4**	0.731
Thiazole-Cu@4CO	0.356	**Thiazole-Cu@4CO_2**	--------	**Thiazole-Cu@4CH_4**	0.726

Oxazole-O System

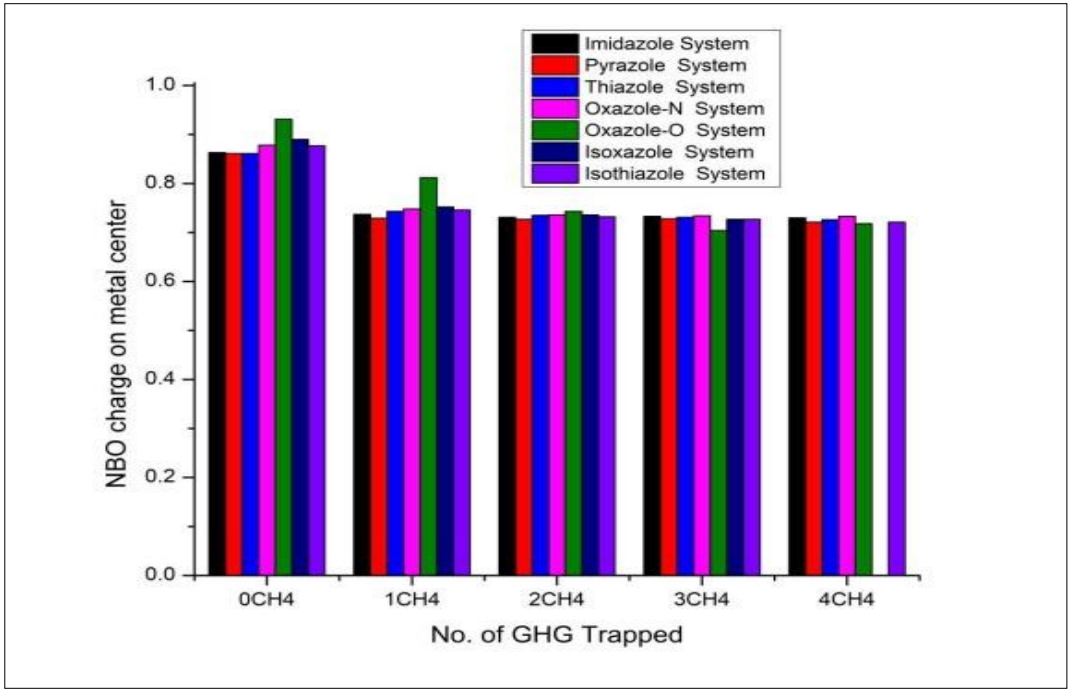
System	NBO	System	NBO	System	NBO
Oxazole-O-Cu	0.931	**Oxazole-O-Cu**	0.931	**Oxazole-O-Cu**	0.931
Oxazole-O-Cu @1CO	0.710	**Oxazole-O-Cu @1CO_2**	0.841	**Oxazole-O-Cu @1CH_4**	0.812
Oxazole-O-Cu @2CO	0.427	**Oxazole-O-Cu @2CO_2**	0.820	**Oxazole-O-Cu @2CH_4**	0.743
Oxazole-O-Cu @3CO	0.102	**Oxazole-O-Cu @3CO_2**	0.772	**Oxazole-O-Cu @3CH_4**	0.704
Oxazole-O-Cu @4 CO	0.424	**Oxazole-O-Cu @ 4 CO_2**	0.775	**Oxazole-O-Cu @4CH_4**	0.718

Oxazole-N System

System	NBO	System	NBO	System	NBO
Oxazole-N-Cu	0.878	**Oxazole-N-Cu**	0.878	**Oxazole-N-Cu**	0.878
Oxazole-N-Cu @1CO	0.636	**Oxazole-N-Cu @1CO_2**	0.773	**Oxazole-N-Cu @1CH_4**	0.748
Oxazole-N-Cu @2CO	0.634	**Oxazole-N-Cu @2CO_2**	0.766	**Oxazole-N-Cu @2CH_4**	0.736
Oxazole-N-Cu @3CO	-0.020	**Oxazole-N-Cu @3CO_2**	0.756	**Oxazole-N-Cu @3CH_4**	0.734
Oxazole-N-Cu @4CO	0.357	**Oxazole-N-Cu @4CO_2**	0.748	**Oxazole-N-Cu @4CH_4**	0.733

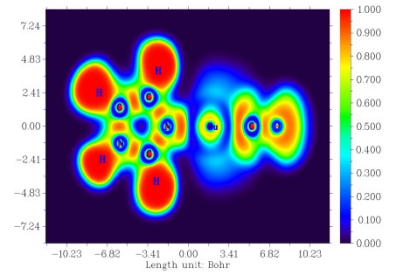

Imidazole System
Pyrazole System
Thiazole System
Oxazole-N System
Oxazole-O System
Isoxazole System
Isothiazole System
NBO Charges on metal center
1.0
0.8
0.6
0.4
0.2
0.0
0CO
1CO
2CO
3CO
4CO
No. of GHG Trapped

[A]

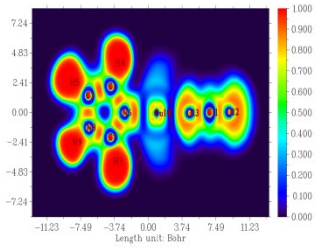


[B]

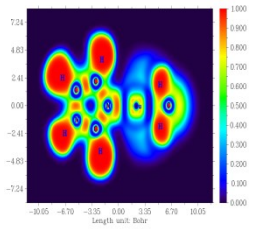
Fig. SF3. *Variation of NBO charges on Cu center in hosts and their sequential different GHGs adsorb systems([A] for CO, and [B] for CH_4).*



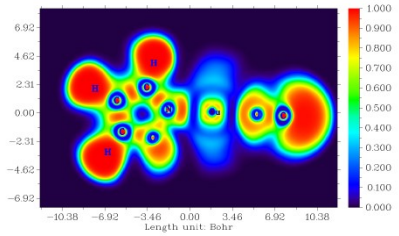
Imidazole-Cu@1CO



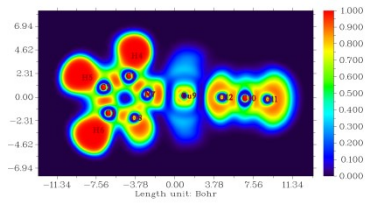
Imidazole-Cu@1CO_2



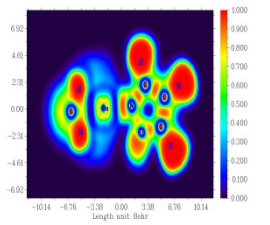
Imidazole-Cu@1CH_4



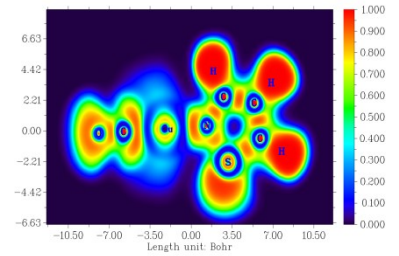
Isoxazole-Cu1CO



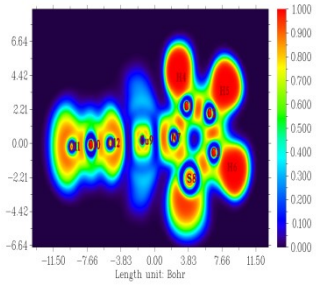
Isoxazole-Cu1CO_2



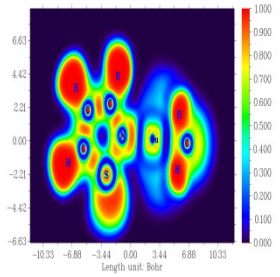
Isoxazole-Cu1CH_4



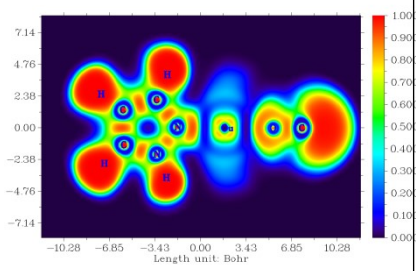
Isothiazole-Cu@1CO



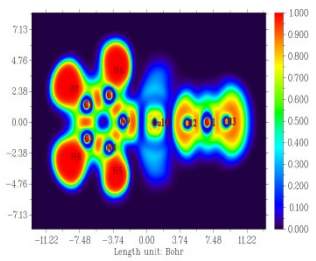
Isothiazole-Cu@1CO_2



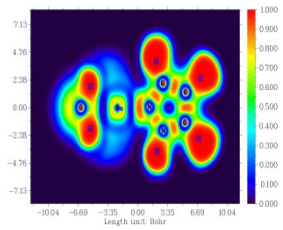
Isothiazole-Cu@1CH_4



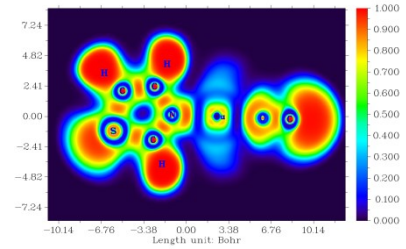
Pyrazole-Cu@1CO



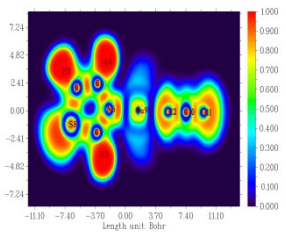
Pyrazole-Cu@1CO_2



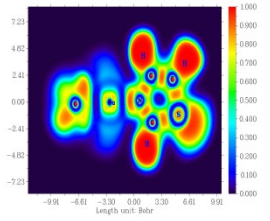
Pyrazole-Cu@1CH_4



Thiazole-Cu@1CO



Thiazole-Cu@1CO_2



Thiazole-Cu@1CH_4

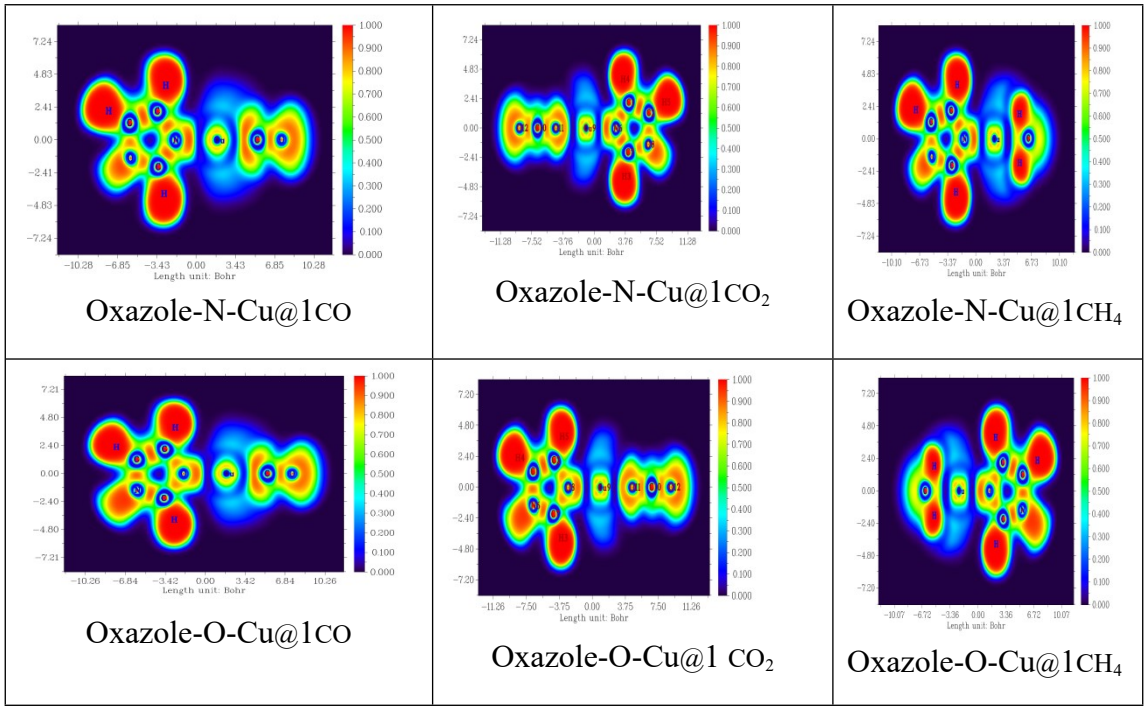


Fig. SF4. ELF plot of different GHGs adsorb different model systems decorated with Cu(I) at B3LYP/6–31+g (d, p) level of theory.