

Table 1

The  $\text{CuCo}_2\text{O}_4$  crystal parameter comparison of computed results and experimental results

	Coarse	Medium	Fine	Shima <sup>1</sup>	Yogesh Sharma <sup>2</sup>	$\text{Cu}_{0.95}\text{Co}_{2.05}\text{O}_4$
$\text{CuCo}_2\text{O}_4$						
a	8.14118	8.14118	8.14118	8.154	8.129	8.133
V	539.588	539.588	539.588			537.96
Density	6.04179	6.04179	6.04179			6.053
HgO						
Hg-O	1.94 Å	1.95 Å	1.95 Å			2.05 Å <sup>3</sup>

<sup>1</sup> M. Shimada, Mater. Res. Bull. 10 (1975) 733.

<sup>2</sup> N.S. Yogesh Sharma, G.V. Subba Rao, V. R. Chowdari, J. Power Sour. 173 (2007) 495.

<sup>3</sup> M. Filatov, D. Cremer, ChemPhysChem 5 (2004) 1547.

TABLE 2. The adsorption energy of mercury on different N-doped slab

	$\Delta E_{\text{ad}}$ (eV)	$\Delta E_{\text{HgO}}$ (eV)	$E_a$ (eV)	$E_a^{-1}$ (eV)
$\text{CuCo}_2\text{O}_4(110)$	0.28	2.61	0.85	0.28
$\text{CuCo}_2\text{O}_3\text{Nb}(110)$	0.22	2.3	0.76	0.21
$\text{CuCo}_2\text{O}_2\text{NbNb}(110)$	0.16	2.08	0.69	0.13

Table 3

The occupancy and hybridization of the calculated natural bond orbital (NBO) for different adsorption system

	<b>NBO</b>	<b>Occupancy</b>	<b>Hybrids</b>
Hg+CuCo <sub>2</sub> O <sub>4</sub> (110)	LP(6)Hg	1.99997	6s
Hg-CuCo <sub>2</sub> O <sub>4</sub> (110)	BD(1)Co <sub>1</sub> -Hg	1.92358	0.2698(sp <sup>0.32</sup> d <sup>0.51</sup> ) <sub>Co</sub> +0.9629(6s) <sub>Hg</sub>
	BD*(1)Co <sub>1</sub> -Hg	0.18465	0.9629(sp <sup>0.32</sup> d <sup>0.51</sup> ) <sub>Co</sub> -0.2698 (s) <sub>Hg</sub>
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>b</sub> (110)	BD(1)Co <sub>1</sub> -Hg( $\alpha$ )	0.96348	0.2774 (sp <sup>0.35</sup> d <sup>0.69</sup> ) <sub>Co</sub> +0.9608(S) <sub>Hg</sub>
	LP(6)Hg( $\beta$ )	0.91818	6s
	BD*(1)Co <sub>1</sub> -Hg( $\alpha$ )	0.13659	0.9608(sp <sup>0.35</sup> d <sup>0.69</sup> ) <sub>Co</sub> -0.2774(s) <sub>Hg</sub>
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>w</sub> (110)	LP(6)Hg( $\alpha$ )	0.92406	6s
	LP(6)Hg( $\beta$ )	0.79850	6s
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>s</sub> (110)	LP(6)Hg( $\alpha$ )	0.88516	6s
	BD(1)Co <sub>1</sub> -Hg( $\beta$ )	0.96879	0.3156(sd <sup>0.37</sup> ) <sub>Co</sub> +0.9489(6s) <sub>Hg</sub>
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>bb</sub> (110)	LP(6)Hg	1.95227	Sd <sup>0.12</sup>
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>bs</sub> (110)	LP(6)Hg	1.77498	6s
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>bw</sub> (110)	LP(6)Hg	1.75885	6s
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>bbs</sub> (110)	LP(6)Hg( $\alpha$ )	0.96306	6sd <sup>0.09</sup>
	LP(6)Hg( $\beta$ )	0.96547	6sd <sup>0.09</sup>
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>bbw</sub> (110)	LP(6)Hg( $\alpha$ )	0.93975	6s
	LP(6)Hg( $\beta$ )	0.88261	6s

Table 4

The second order perturbation stabilization energies E(2) for the systems

	<b>Donor NBO(i)</b>	<b>Acceptor NBO(j)</b>	<b>E(2) (Kcal/mol)</b>
Hg+CuCo <sub>2</sub> O <sub>4</sub> (110)			
Hg-CuCo <sub>2</sub> O <sub>4</sub> (110)	BD (1)Co <sub>1</sub> -O <sub>1</sub>	BD*(1)Co <sub>1</sub> -Hg	45.13
	BD(1)Co <sub>1</sub> -O <sub>2</sub>	BD*(1)Co <sub>1</sub> -Hg	45.80
	BD(1)Co <sub>1</sub> -Hg	BD*(1)Co <sub>1</sub> -O <sub>1</sub>	17.78
	BD (1)Co <sub>1</sub> -Hg	BD*(1)Co <sub>1</sub> -O <sub>2</sub>	17.94
	BD(1)Co <sub>1</sub> -Hg	BD*(1)Co <sub>1</sub> -O <sub>w</sub>	5.72
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>bb</sub> (110)	LP(6)Hg	BD*(1)Co <sub>1</sub> -N <sub>b1</sub>	10.16
	LP(6)Hg	BD*(1)Co <sub>1</sub> -N <sub>b2</sub>	9.88
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>bs</sub> (110)	LP(6)Hg	BD*(1)Co <sub>1</sub> -N <sub>b1</sub>	18.32
	LP(6)Hg	BD*(1)Co <sub>1</sub> -O <sub>2</sub>	22.14
	LP(6)Hg	BD*(1)Co <sub>1</sub> -O <sub>w</sub>	5.53
Hg-CuCo <sub>2</sub> O <sub>4</sub> N <sub>bw</sub> (110)	LP(6)Hg	BD*(1)Co <sub>1</sub> -N <sub>b1</sub>	21.58
	LP(6)Hg	BD*(1)Co <sub>1</sub> -O <sub>2</sub>	22.98
	LP(6)Hg	BD*(1)Co <sub>1</sub> -N <sub>w</sub>	7.13



M1'

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XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
  x Element      Atom      Fractional coordinates of atoms  x
  x              Number      u          v          w
  x-----x
  x O           1           0.284920  0.500000  0.011360
  x O           2           0.809419  0.000314  0.147752
  x O           3           0.784920  1.000000  0.000000
  x O           4           0.291993  0.500442  0.136708
  x O           5           0.515140  0.270017  0.073102
  x O           6           0.265080  0.000000  0.011360
  x O           7           0.254934  1.000073  0.137145
  x O           8           0.765080  0.500000  0.000000
  x O           9           0.048924  0.770192  0.073204
  x O          10           0.629470  0.504389  0.209308
  x O          11           0.049370  0.230061  0.073163
  x O          12           0.514823  0.730791  0.072964
  x Co           1           0.515148  0.501426  0.140909
  x Co           2           0.025000  1.000000  0.005680
  x Co           3           0.021239  0.000316  0.137736
  x Co           4           0.525000  0.500000  0.005680
  x Co           5           0.280383  0.752410  0.074015
  x Co           6           0.280843  0.247846  0.074049
  x Cu           1           0.667246  0.000583  0.076642
  x Cu           2           0.923945  0.499948  0.057830
  x Hg           1           0.788003  0.499743  0.315108
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XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
  x Element      Atom      Fractional coordinates of atoms  x
  x              Number      u          v          w
  x-----x
  x O           1           0.284920  0.500000  0.011360
  x O           2           0.807572 -0.000332  0.147845
  x O           3           0.784920  1.000000  0.000000
  x O           4           0.284271  0.499892  0.136066
  x O           5           0.513662  0.276923  0.074579
  x O           6           0.265080  0.000000  0.011360
  x O           7           0.251708  1.000059  0.137081
  x O           8           0.765080  0.500000  0.000000
  x O           9           0.047079  0.770488  0.073095
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x	O	10	0.576072	0.503923	0.224587
x	O	11	0.047238	0.229678	0.073085
x	O	12	0.513691	0.721232	0.075385
x	Co	1	0.506292	0.499068	0.146721
x	Co	2	0.025000	1.000000	0.005680
x	Co	3	0.019267	0.000189	0.137915
x	Co	4	0.525000	0.500000	0.005680
x	Co	5	0.278992	0.751638	0.074050
x	Co	6	0.279228	0.248300	0.073976
x	Cu	1	0.665603	-0.000580	0.076429
x	Cu	2	0.924204	0.500029	0.057486
x	Hg	1	0.502147	0.504825	0.346160

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(Hg-O<sub>w</sub>)<sub>TS</sub>

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Coordinates: Fractional components

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Element	Atom Number	x	y	z
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O	1	0.284919	0.499999	0.011360
O	2	0.810192	0.000232	0.147246
O	3	0.784918	0.999997	0.000000
O	4	0.295614	0.500203	0.136270
O	5	0.512455	0.267347	0.072294
O	6	0.265080	0.000000	0.011360
O	7	0.253021	1.000051	0.137005
O	8	0.765079	0.499999	0.000000
O	9	0.046351	0.768280	0.072680
O	10	0.696488	0.502259	0.181143
O	11	0.046590	0.231870	0.072655
O	12	0.512293	0.733062	0.072223
Co	1	0.520356	0.500711	0.138703
Co	2	0.025000	0.999997	0.005680

Co	3	0.021640	0.000176	0.137133
Co	4	0.524999	0.499999	0.005680
Co	5	0.278582	0.751467	0.073756
Co	6	0.278822	0.248654	0.073771
Cu	1	0.666310	0.000301	0.076298
Cu	2	0.906080	0.499964	0.066500
Hg	1	0.653264	0.499574	0.308654

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(Hg-O<sub>s</sub>)<sub>TS</sub>

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Coordinates: Fractional components

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Element	Atom Number	x	y	z
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O	1	0.284919	0.499999	0.011360
O	2	0.808138	0.000010	0.146857
O	3	0.784918	0.999997	0.000000
O	4	0.378747	0.499857	0.193218
O	5	0.507978	0.264735	0.071520
O	6	0.265080	0.000000	0.011360
O	7	0.248828	1.000008	0.135904
O	8	0.765079	0.499999	0.000000
O	9	0.043206	0.763498	0.071923
O	10	0.743520	0.500168	0.145942
O	11	0.043212	0.236504	0.071923
O	12	0.507972	0.735278	0.071515
Co	1	0.531063	0.500031	0.135961
Co	2	0.025000	0.999997	0.005680
Co	3	0.018954	-0.000001	0.135776
Co	4	0.524999	0.499999	0.005680
Co	5	0.276683	0.753010	0.072040
Co	6	0.276694	0.246969	0.072034

Cu	1	0.664720	-0.000004	0.075546
Cu	2	0.887943	0.499998	0.074601
Hg	1	0.256847	0.500051	0.311936

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Hg<sub>a</sub>: Hg adsorb on CuCoO<sub>4</sub>-N<sub>b</sub>(110)

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x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	
x-----x						
x	N	1	0.512916	0.261366	0.066352	
x	O	1	0.284920	0.500000	0.011360	
x	O	2	0.811049	-0.031685	0.146826	
x	O	3	0.784920	1.000000	0.000000	
x	O	4	0.293871	0.502012	0.136325	
x	O	5	0.265080	0.000000	0.011360	
x	O	6	0.250801	1.000871	0.136345	
x	O	7	0.765080	0.500000	0.000000	
x	O	8	0.043335	0.765104	0.071462	
x	O	9	0.737954	0.481876	0.144719	
x	O	10	0.038192	0.232316	0.071833	
x	O	11	0.508473	0.724564	0.072818	
x	Co	1	0.525132	0.477107	0.134810	
x	Co	2	0.025000	1.000000	0.005680	
x	Co	3	0.021815	-0.001093	0.135927	
x	Co	4	0.525000	0.500000	0.005680	
x	Co	5	0.275711	0.748152	0.073470	
x	Co	6	0.287104	0.248342	0.073722	
x	Cu	1	0.668335	0.026483	0.078389	
x	Cu	2	0.885620	0.497768	0.075010	
x	Hg	1	0.520671	0.454679	0.276818	

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x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	
x-----x						
x	N	1	0.514552	0.266510	0.069663	

x	O	1	0.284920	0.500000	0.011360
x	O	2	0.812301	-0.032702	0.147144
x	O	3	0.784920	1.000000	0.000000
x	O	4	0.290134	0.501229	0.136809
x	O	5	0.265080	0.000000	0.011360
x	O	6	0.254674	1.002362	0.136552
x	O	7	0.765080	0.500000	0.000000
x	O	8	0.050256	0.770307	0.072540
x	O	9	0.630016	0.482187	0.206668
x	O	10	0.040811	0.229499	0.073154
x	O	11	0.514176	0.722076	0.073309
x	Co	1	0.513844	0.484488	0.138616
x	Co	2	0.025000	1.000000	0.005680
x	Co	3	0.023544	-0.001475	0.137573
x	Co	4	0.525000	0.500000	0.005680
x	Co	5	0.281123	0.750944	0.074080
x	Co	6	0.286848	0.247742	0.073168
x	Cu	1	0.671627	0.033433	0.079118
x	Cu	2	0.921460	0.502712	0.059269
x	Hg	1	0.784564	0.453071	0.317251

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TS(Hg-O<sub>w</sub>)<sub>N</sub>

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Coordinates: Fractional components

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Element	Atom Number	x	y	z
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N	1	0.514038	0.263956	0.068103
O	1	0.284919	0.499999	0.011360
O	2	0.812812	-0.031710	0.147006
O	3	0.784918	0.999997	0.000000
O	4	0.291351	0.501699	0.136693
O	5	0.265080	0.000000	0.011360
O	6	0.253808	1.001575	0.136621



O	7	0.765079	0.499999	0.000000
O	8	0.047466	0.768440	0.072133
O	9	0.692912	0.482533	0.179660
O	10	0.040161	0.230261	0.072610
O	11	0.511635	0.723585	0.073045
Co	1	0.517032	0.480827	0.136501
Co	2	0.025000	0.999997	0.005680
Co	3	0.023697	-0.001254	0.137026
Co	4	0.524999	0.499999	0.005680
Co	5	0.278871	0.749717	0.073849
Co	6	0.287174	0.247952	0.073439
Cu	1	0.670438	0.030029	0.078966
Cu	2	0.904117	0.500541	0.067509
Hg	1	0.648967	0.451090	0.310132

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H<sub>a</sub>: Hg adsorb on CuCoO<sub>4</sub>-N<sub>bb</sub>(110)

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x	Element	Atom Number	Fractional coordinates of atoms		
			u	v	w
x	N	1	0.513729	0.273489	0.071497
x	N	2	0.513725	0.726523	0.071492
x	O	1	0.284920	0.500000	0.011360
x	O	2	0.805587	0.000007	0.148032
x	O	3	0.784920	1.000000	0.000000
x	O	4	0.304628	0.499996	0.136073
x	O	5	0.265080	0.000000	0.011360
x	O	6	0.247662	1.000000	0.136635
x	O	7	0.765080	0.500000	0.000000
x	O	8	0.037756	0.766288	0.071418
x	O	9	0.749763	0.500024	0.145912
x	O	10	0.037755	0.233704	0.071418
x	Co	1	0.537062	0.500016	0.135965
x	Co	2	0.025000	1.000000	0.005680
x	Co	3	0.015895	0.000000	0.134132
x	Co	4	0.525000	0.500000	0.005680
x	Co	5	0.287158	0.753535	0.073518
x	Co	6	0.287162	0.246462	0.073518
x	Cu	1	0.655762	0.000007	0.075079
x	Cu	2	0.888656	0.499999	0.073791

x Hg 1 0.529227 0.500050 0.280448

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x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	
x	N	1	0.516405	0.269191	0.071498	
x	N	2	0.516151	0.730613	0.071444	
x	O	1	0.284920	0.500000	0.011360	
x	O	2	0.810253	-0.000120	0.147195	
x	O	3	0.784920	1.000000	0.000000	
x	O	4	0.292401	0.499936	0.137118	
x	O	5	0.265080	0.000000	0.011360	
x	O	6	0.253324	0.999836	0.136324	
x	O	7	0.765080	0.500000	0.000000	
x	O	8	0.042246	0.770439	0.072729	
x	O	9	0.647454	0.504465	0.199802	
x	O	10	0.042333	0.229256	0.072743	
x	Co	1	0.517299	0.500300	0.136158	
x	Co	2	0.025000	1.000000	0.005680	
x	Co	3	0.021215	-0.000202	0.136962	
x	Co	4	0.525000	0.500000	0.005680	
x	Co	5	0.287782	0.751413	0.073564	
x	Co	6	0.288045	0.248463	0.073586	
x	Cu	1	0.660833	-0.000256	0.076761	
x	Cu	2	0.923049	0.499776	0.058177	
x	Hg	1	0.773821	0.499847	0.321069	

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TS(Hg-O<sub>w</sub>)<sub>2N</sub>

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Coordinates: Fractional components

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Element      Atom
             Number      x          y          z
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N            1            0.515515  0.270736  0.071336
N            2            0.515366  0.729132  0.071310
O            1            0.284919  0.499999  0.011360
O            2            0.809119 -0.000009  0.147362
O            3            0.784918  0.999997  0.000000
O            4            0.297042  0.499960  0.136870
O            5            0.265080  0.000000  0.011360
O            6            0.251763  0.999900  0.136559
O            7            0.765079  0.499999  0.000000
O            8            0.041026  0.769202  0.072235
O            9            0.697080  0.502582  0.180333
O           10            0.041076  0.230629  0.072239
Co           1            0.523603  0.500161  0.135786
Co           2            0.025000  0.999997  0.005680
Co           3            0.019686 -0.000105  0.135986
Co           4            0.524999  0.499999  0.005680
Co           5            0.287813  0.752355  0.073598
Co           6            0.287964  0.247567  0.073610
Cu           1            0.658999 -0.000156  0.076069
Cu           2            0.909351  0.499873  0.064821
Hg           1            0.671510  0.499740  0.314964
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H<sub>a</sub>: Hg adsorb on CuCoO<sub>4</sub>-N<sub>bbs</sub>(110)

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x	Element	Atom	Fractional coordinates of atoms		
x		Number	u	v	w
x	N	1	0.510648	0.265495	0.067703
x	N	2	0.510675	0.734457	0.067723
x	N	3	0.276534	0.499992	0.138802

x	O	1	0.284920	0.500000	0.011360
x	O	2	0.805129	-0.000013	0.146050
x	O	3	0.784920	1.000000	0.000000
x	O	4	0.265080	0.000000	0.011360
x	O	5	0.246172	0.999992	0.136913
x	O	6	0.765080	0.500000	0.000000
x	O	7	0.035509	0.765263	0.071052
x	O	8	0.721609	0.499778	0.145835
x	O	9	0.035524	0.234735	0.071051
x	Co	1	0.506308	0.499919	0.131523
x	Co	2	0.025000	1.000000	0.005680
x	Co	3	0.016381	-0.000008	0.134387
x	Co	4	0.525000	0.500000	0.005680
x	Co	5	0.285006	0.743319	0.076990
x	Co	6	0.284995	0.256684	0.076991
x	Cu	1	0.655900	0.000014	0.074326
x	Cu	2	0.876465	0.500043	0.077703
x	Hg	1	0.498539	0.499969	0.275667

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M4

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x	Element	Atom	Fractional coordinates of atoms			x
x		Number	u	v	w	
x	N	1	0.514177	0.271672	0.070754	
x	N	2	0.514222	0.725242	0.071622	
x	N	3	0.271106	0.499075	0.139187	
x	O	1	0.284920	0.500000	0.011360	
x	O	2	0.808894	-0.001278	0.147127	
x	O	3	0.784920	1.000000	0.000000	
x	O	4	0.265080	0.000000	0.011360	
x	O	5	0.250794	0.999640	0.136426	
x	O	6	0.765080	0.500000	0.000000	
x	O	7	0.039068	0.770403	0.072503	
x	O	8	0.630587	0.494305	0.198136	
x	O	9	0.038979	0.229466	0.072611	
x	Co	1	0.489996	0.496327	0.137479	
x	Co	2	0.025000	1.000000	0.005680	
x	Co	3	0.020290	-0.000208	0.137043	

