Electronic Supporting Information

A comparative study of Cu_nX (X=Sc, Y; n=1-10) clusters based on structures, electronic and aromatic properties

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Cartesian cordialities for the lowest-energy structures and low-lying isomers are listed in the paper.

CuSc Cluster

Cu	0.00000000	0.00000000	1.07655600
Sc	0.00000000	0.00000000	-1.48667300

Cu_2Sc Cluster

Cu	0.00000000	2.58438300	-0.00009900
Cu	0.00000000	-2.58438300	-0.00009900
Sc	0.00000000	0.00000000	0.00027300

Cu_3Sc Cluster

Cu	0.00000000	0.00000000	1.11478700
Cu	0.00000000	2.14581100	0.01490300
Cu	0.00000000	-2.14581100	0.01490300
Sc	0.00000000	0.00000000	-1.58062800

Cu_4Sc Cluster

Cu	-0.06109000	1.27363200	1.20819100
Cu	-0.06109000	-0.90299900	-2.55185600
Cu	-0.06109000	-0.90299900	2.55185600
Cu	-0.06109000	1.27363200	-1.20819100
Sc	0.33745000	-1.02365300	0.00000000

Cu_5Sc Cluster

Cu	0.03910900	-0.95513100	2.11405600
Cu	0.03910900	-0.95513100	-2.11405600
Cu	0.03910900	1.38447100	1.19303000
Cu	0.03910900	1.38447100	-1.19303000
Cu	-1.21892500	-0.49315700	0.00000000
Sc	1.46724900	-0.50476900	0.00000000

Cu_6Sc Cluster

Cu	2.45881700	-0.02568700	0.49136900
Cu	-1.28474300	2.07632100	0.49563000
Cu	-1.33602500	0.01477300	-0.96859100
Cu	0.73512200	-1.27110300	-0.79990500
Cu	0.76330100	1.25189300	-0.80339000

Cu	-1.33391700	-2.04606500	0.49507700
Sc	-0.00352800	-0.00018300	1.50497700

Cu_7Sc Cluster

Cu	0.00000000	2.75394747	-0.00000000
Cu	2.15312283	1.71705816	-0.00000000
Cu	2.68490026	-0.61281097	-0.00000000
Cu	-1.19489302	-2.48122093	-0.00000000
Cu	-2.68490026	-0.61281096	-0.00000000
Cu	-2.15312283	1.71705816	-0.00000000
Cu	1.19489302	-2.48122093	-0.00000000
Sc	-0.00000000	-0.00000000	-0.00000000

Cu_8Sc Cluster

Cu	-2.22473800	1.35454000	0.58098100
Cu	-2.22473800	-1.35454000	0.58098100
Cu	0.00000000	2.10155000	-0.33859800
Cu	-1.22362200	0.00000000	-1.26614100
Cu	2.22473800	1.35454000	0.58098100
Cu	1.22362200	0.00000000	-1.26614100
Cu	0.00000000	-2.10155000	-0.33859800
Cu	2.22473800	-1.35454000	0.58098100
Sc	0.00000000	0.00000000	1.22290600

Cu_9Sc Cluster

Cu	-2.31400100	1.33598900	0.84088100
Cu	0.00000000	2.46578300	0.16329800
Cu	2.31400100	1.33598900	0.84088100
Cu	-2.13543000	-1.23289100	0.16329800
Cu	0.00000000	-1.44343300	-1.26670200
Cu	1.25004900	0.72171600	-1.26670200
Cu	2.13543000	-1.23289100	0.16329800
Cu	0.00000000	-2.67197800	0.84088100
Cu	-1.25004900	0.72171600	-1.26670200
Sc	0.00000000	0.00000000	1.08759700

$Cu_{10}Sc$ Cluster

Cu	-0.59436200	-1.28756500	1.45456900
Cu	1.40518100	-1.48247700	0.00000000
Cu	-0.59436200	-1.28756500	-1.45456900

Cu	-2.48243900	0.39295500	-1.21113900
Cu	-2.48243900	0.39295500	1.21113900
Cu	-0.59436200	0.99582300	2.68917500
Cu	1.57103100	0.03625200	2.07028000
Cu	2.81206600	0.58207500	0.00000000
Cu	1.57103100	0.03625200	-2.07028000
Cu	-0.59436200	0.99582300	-2.68917500
Sc	-0.02345500	0.86374400	0.00000000

CuY Cluster

Cu	0.00000000	0.00000000	-1.54915200
Y	0.00000000	0.00000000	1.15193400

Cu_2Y Cluster

Cu	2.44209100	-0.47513800	0.00000000
Cu	-2.44209100	-0.47524100	0.00000000
Y	0.00000000	0.70669200	0.00000000

Cu_3Y Cluster

Cu	0.00000000	2.70323700	0.00000000
Cu	2.34107200	-1.35161800	0.00000000
Cu	-2.34107200	-1.35161800	0.00000000
Y	0.00000000	0.00000000	0.00000000

Cu_4Y Cluster

Cu	0.00000000	2.73977000	0.51914500
Cu	0.00000000	1.18580500	-1.36251300
Cu	0.00000000	-1.18580500	-1.36251300
Cu	0.00000000	-2.73977000	0.51914500
Y	0.00000000	0.00000000	1.25423800

Cu_5Y Cluster

Cu	0.00000000	1.79999400	-0.17906700
Cu	0.00000000	-1.79999400	-0.17906700
Cu	-1.79999400	0.00000000	-0.17906700
Cu	0.00000000	0.00000000	-1.89661100
Cu	1.79999400	0.00000000	-0.17906700
Y	0.00000000	0.00000000	1.94291000

Cu_6Y Cluster

Cu	-0.41686600	-1.32490100	2.09287700
Cu	1.48911000	2.02707800	0.00000000
Cu	-1.63360600	-0.56695700	0.00000000
Cu	-0.41686600	1.12359300	1.28953600
Cu	-0.41686600	-1.32490100	-2.09287700
Cu	-0.41686600	1.12359300	-1.28953600
Y	1.34735500	-0.78634900	0.00000000

Cu_7Y Cluster

Cu	0.00000000	2.83874000	0.00000000
Cu	2.21941600	1.76992500	0.00000000
Cu	1.23168300	-2.55761600	0.00000000
Cu	-2.21941600	1.76992500	0.00000000
Cu	-1.23168300	-2.55761600	0.00000000
Cu	-2.76756700	-0.63167900	0.00000000
Cu	2.76756700	-0.63167900	0.00000000
Y	0.00000000	0.00000000	0.00000000

Cu_8Y Cluster

Cu	-1.38517000	2.27588300	0.42751700
Cu	0.00000000	1.22713400	-1.34837100
Cu	-2.09728300	0.00000000	-0.44650300
Cu	2.09728300	0.00000000	-0.44650300
Cu	-1.38517000	-2.27588300	0.42751700
Cu	1.38517000	-2.27588300	0.42751700
Cu	0.00000000	-1.22713400	-1.34837100
Cu	1.38517000	2.27588300	0.42751700
Y	0.00000000	0.00000000	1.39771100

Cu_9Y Cluster

Cu	-1.24893800	0.72107400	-1.32817100
Cu	0.00000000	2.49905300	0.03702800
Cu	-2.16424300	-1.24952600	0.03702800
Cu	2.16424300	-1.24952600	0.03702800
Cu	1.24893800	0.72107400	-1.32817100
Cu	-2.39156600	1.38077100	0.71417900
Cu	0.00000000	-1.44214900	-1.32817100
Cu	2.39156600	1.38077100	0.71417900
Cu	0.00000000	-2.76154200	0.71417900

Y	0.00000000	0.00000000	1.28707200

$Cu_{10}Y$ Cluster

Cu	-2.02856400	0.42841400	0.00000000
Cu	-0.83988800	-1.19478500	1.42507400
Cu	1.54790300	-2.00274200	-1.23358900
Cu	-0.83988800	-1.19478500	-1.42507400
Cu	1.54790300	-2.00274200	1.23358900
Cu	-0.83988800	1.34768700	2.10848500
Cu	1.06289000	-0.09705400	-2.80110500
Cu	-0.83988800	1.34768700	-2.10848500
Cu	1.06289000	-0.09705400	2.80110500
Cu	-1.08107000	2.72579400	0.00000000
Y	0.92770100	0.54994500	0.00000000

Table S1. Basis set effects on the polarizability ($a_{xx}, a_{yy}, a_{zz}, \bar{a}$) of CuSc and CuY clusters at the B3LYP/MP2 level of theory.

Cluster	Basis set	Functional	a_{xx} (a.u.)	a_{yy}(a.u.)	a_{zz} (a.u.)	$\bar{a}$ (a.u.)
CuSc	Aug-cc-pvtz	B3LYP	146.49	122.19	195.08	154.59
		MP2	164.28	183.67	212.03	186.66
	Lanl2dz	B3LYP	155.84	121.84	199.21	158.96
		MP2	165.31	183.29	241.86	196.82
	6-311+G(d)	B3LYP	145.78	121.32	196.67	154.59
		MP2	161.74	150.54	223.91	178.73
CuY	cc-pvtz-pp	B3LYP	167.19	167.19	191.20	175.19
		MP2	179.77	179.77	221.63	193.72
	Lanl2dz	B3LYP	177.53	177.53	192.12	182.39
		MP2	190.84	190.84	220.89	200.86
	Aug-cc-pvtz	B3LYP	160.62	160.62	187.91	169.71
		MP2	176.51	176.51	217.35	190.12
	Def2-QZVP	B3LYP	159.62	159.62	187.39	168.86
		MP2	175.69	175.69	210.79	187.39

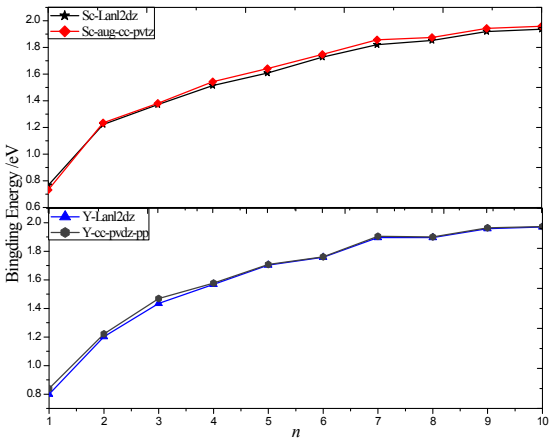


Figure S1. Binding energy (BE) of the Cu_nX (X=Sc, Y; n=1-10) clusters calculated with Lanl2dz, cc-pvdz-pp, aug-cc-pvtz, respectively.

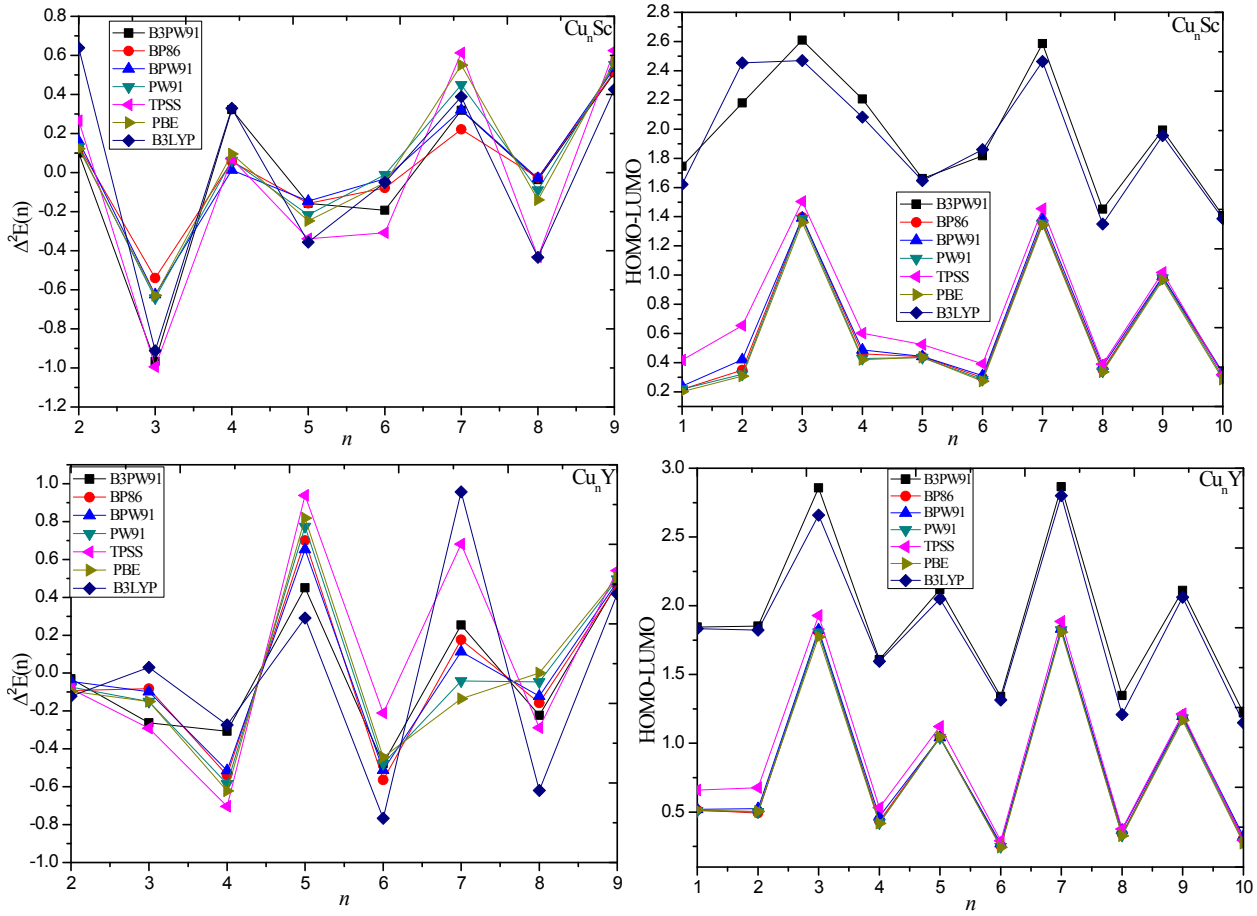
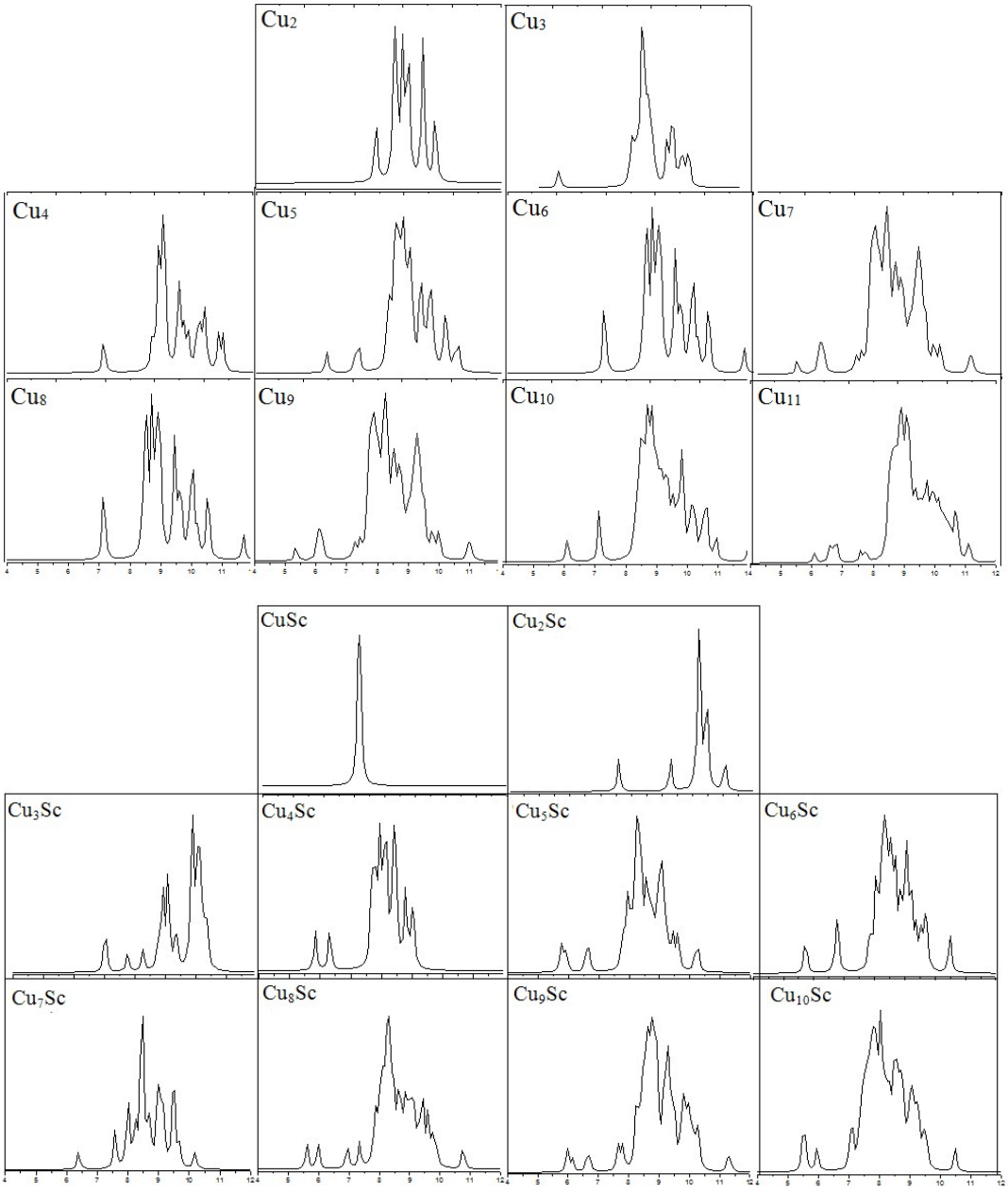


Figure S2. Second-order energy differences (Δ_2E) and HOMO-LUMO energy of the Cu_nX (X=Sc, Y; n=1-10) clusters based on the different density functionals (B3PW91, BP86, BPW91, PBE, PW91 and TPSS).


Cu2
Cu3
Cu4
Cu5
Cu6
Cu7
Cu8
Cu9
Cu10
Cu11
CuSc
Cu2Sc
Cu3Sc
Cu4Sc
Cu5Sc
Cu6Sc
Cu7Sc
Cu8Sc
Cu9Sc
Cu10Sc

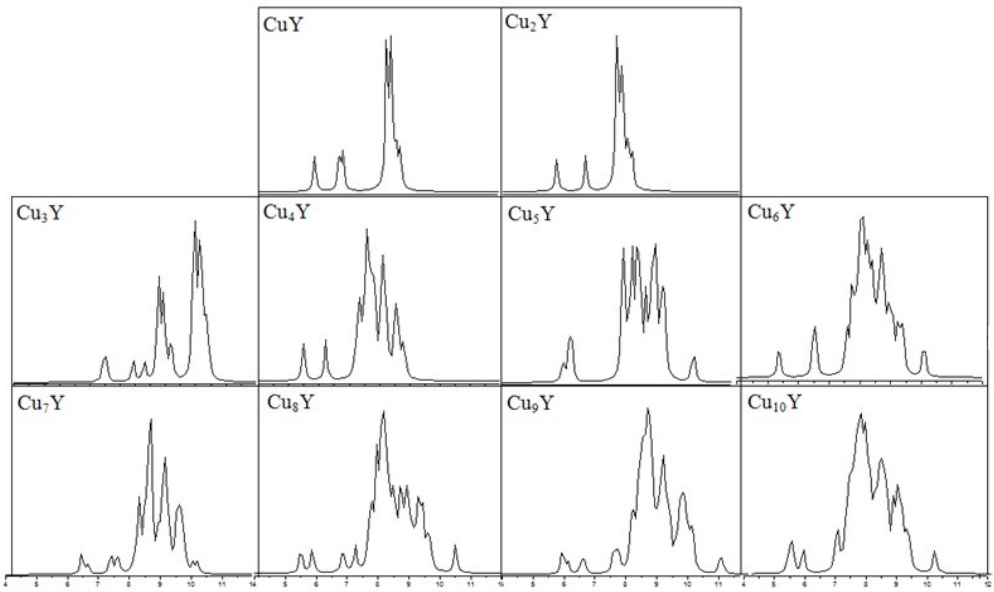


Figure S3. Simulated photoelectron spectra of the lowest energy structures Cu_n and Cu_nX (X=Sc, Y; n=1-10).