

Au_n (n=1-16) clusters on ZrO₂ (111) surface: a DFT+U investigation

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1. The lattice parameters and coordinates of the ZrO₂ (111) surface

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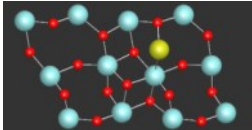
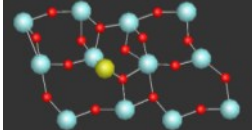
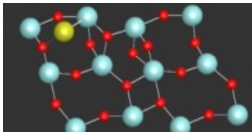
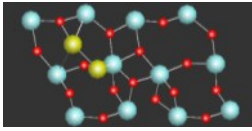
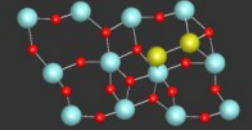
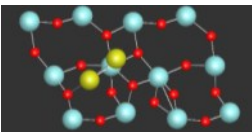
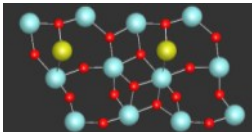
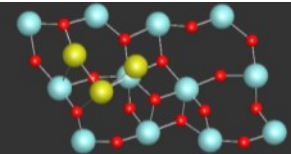
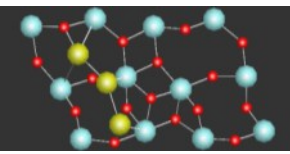
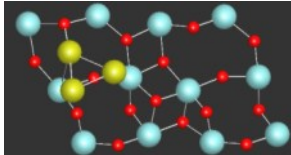
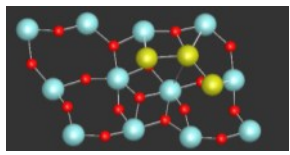
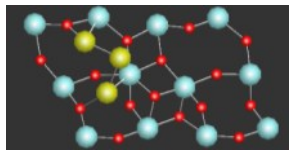
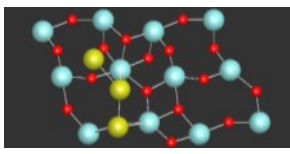
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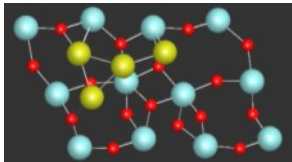
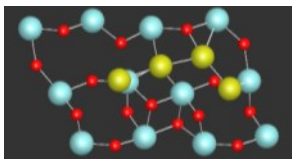
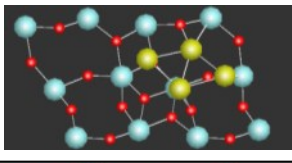
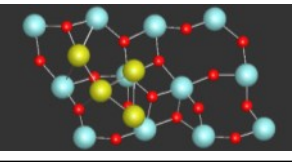
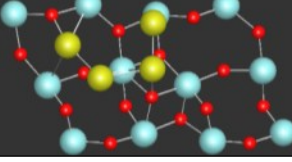
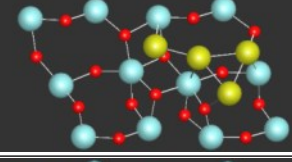
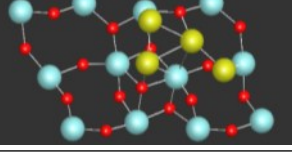
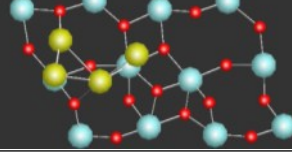
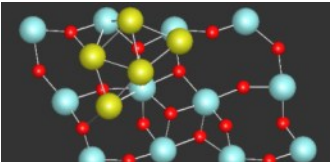
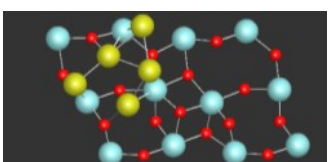
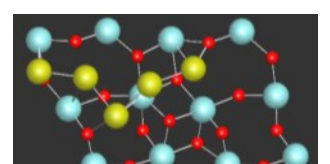
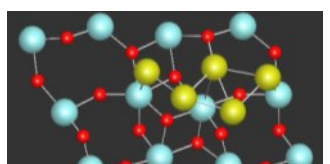
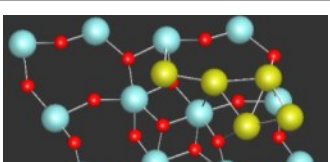
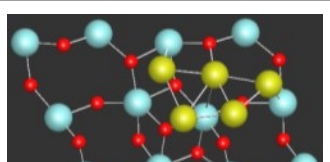
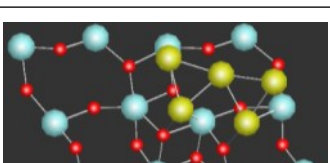
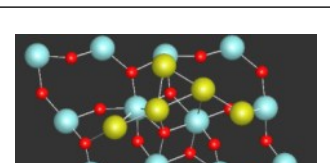
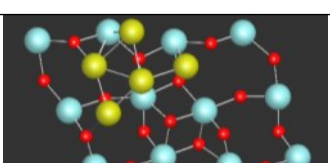
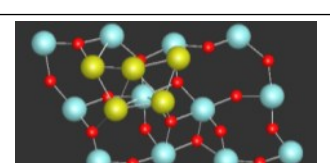
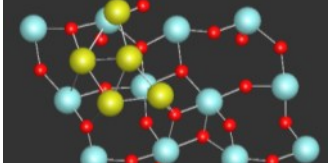
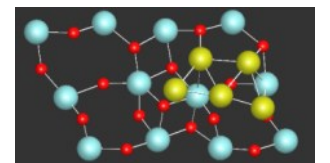
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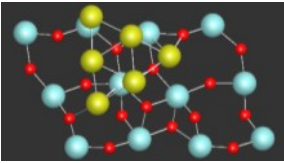
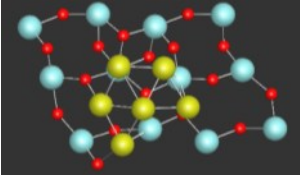
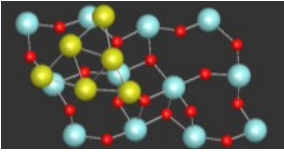
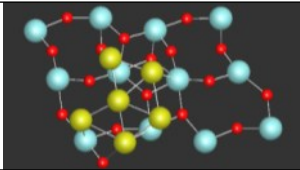
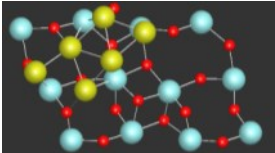
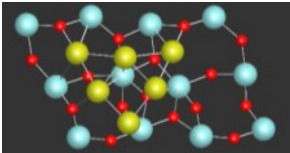
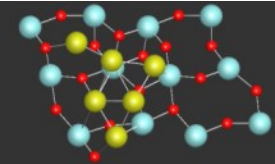
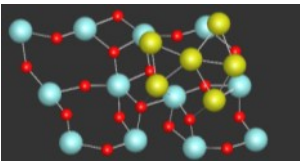
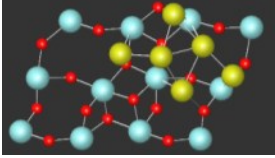
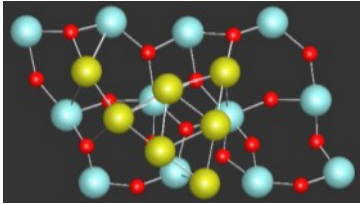
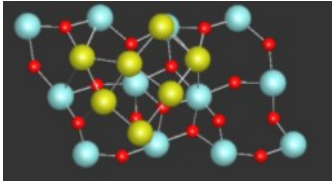
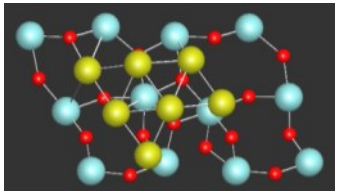
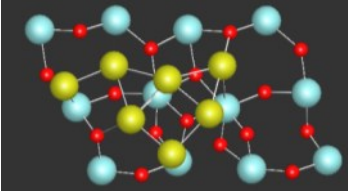
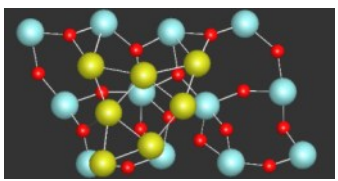
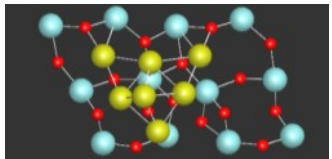
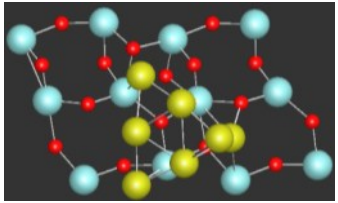
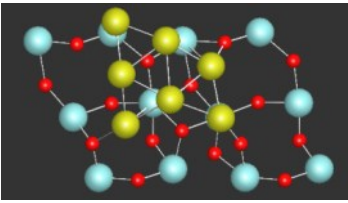
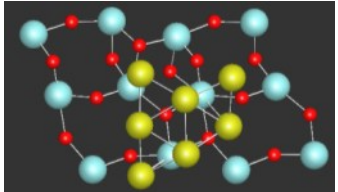
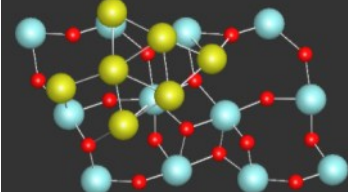
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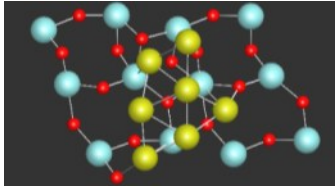
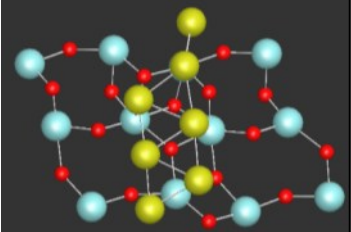
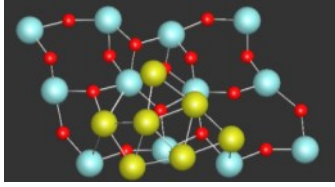
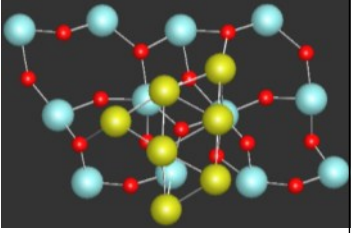
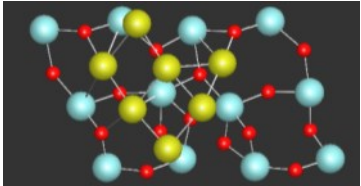
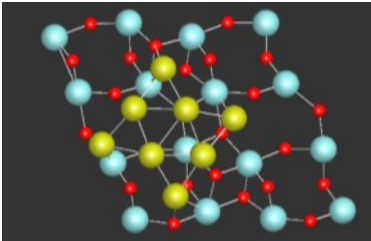
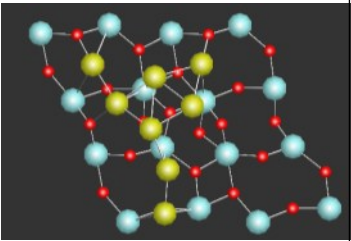
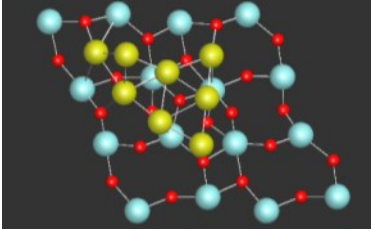
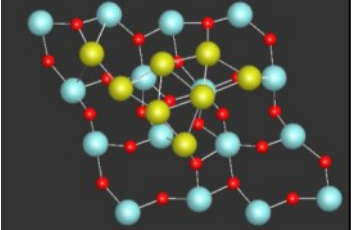
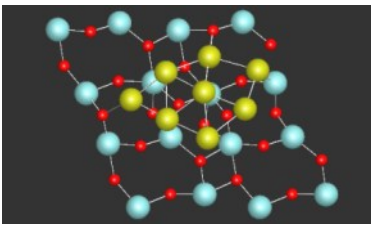
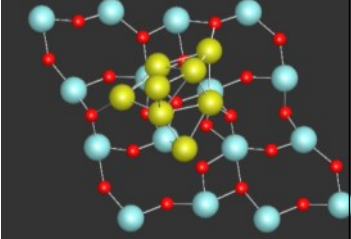
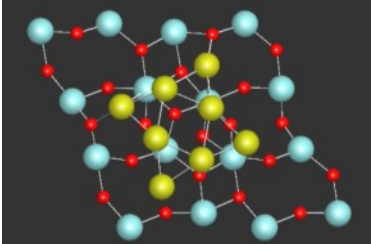
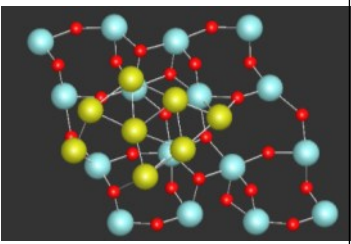
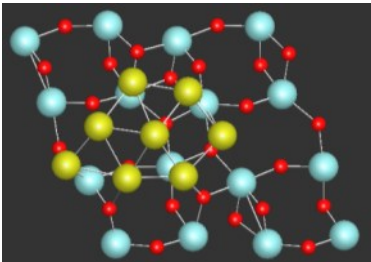
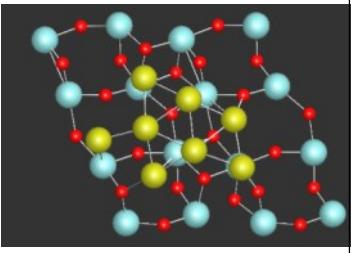
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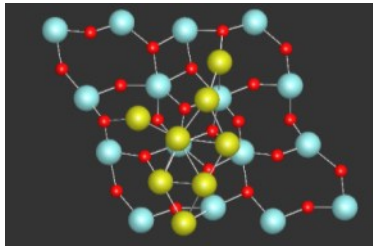
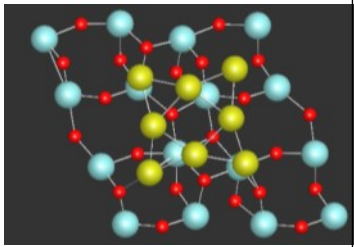
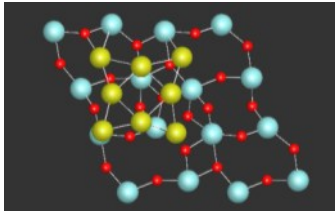
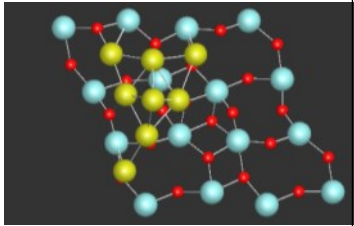
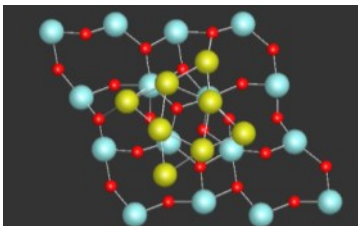
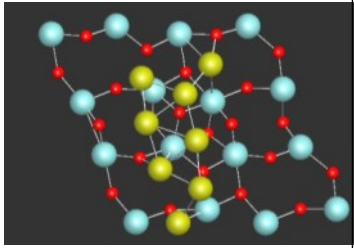
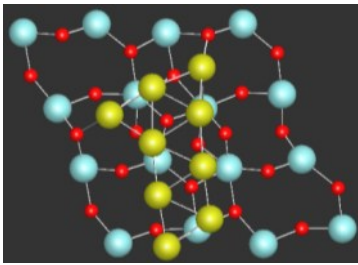
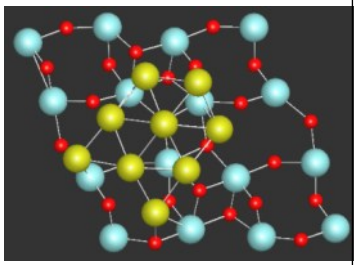
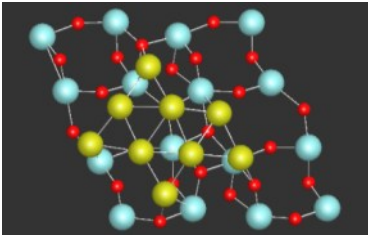
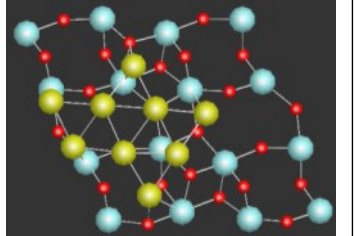
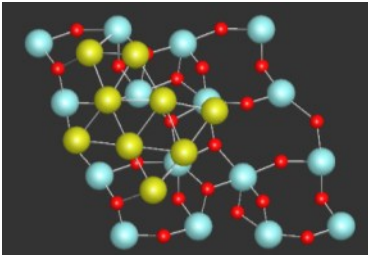
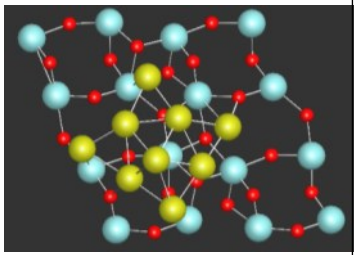
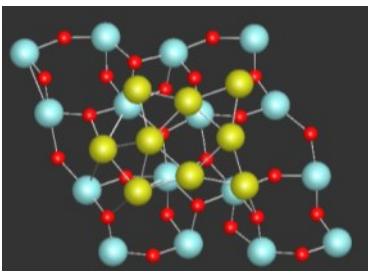
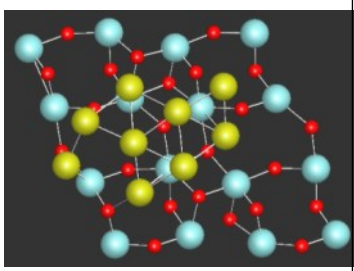
2. The structure and relative energies (E_{rel} , eV) of the considered Au_n/ZrO_2 (Structures with 3D Au_n clusters were labelled in red color.)

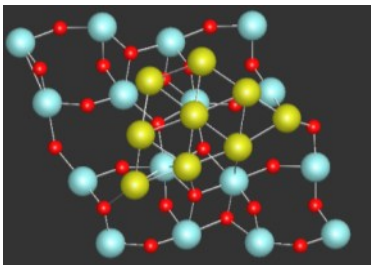
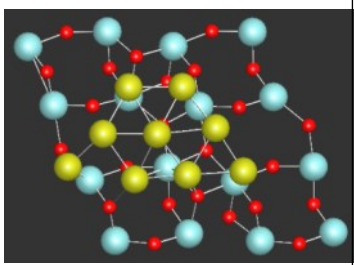
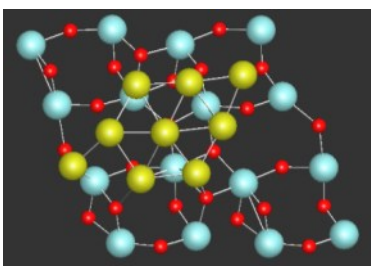
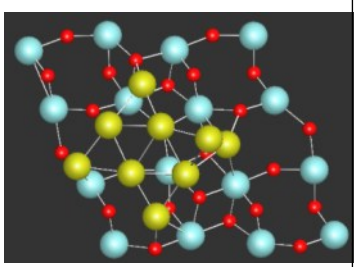
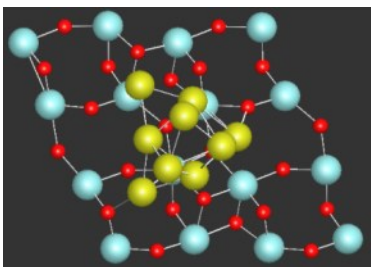
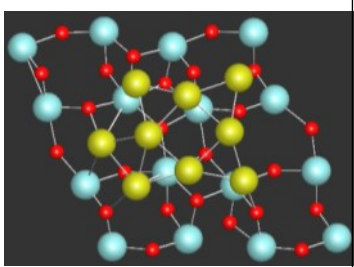
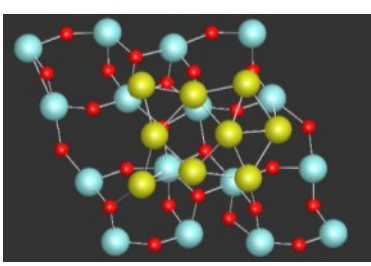
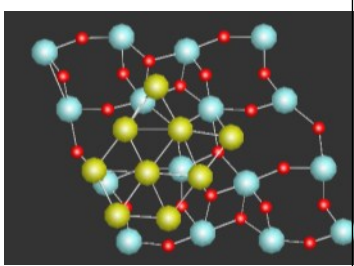
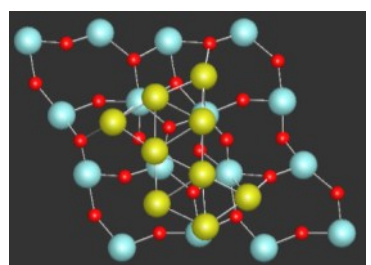
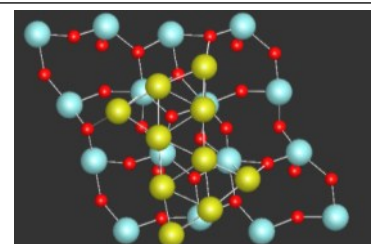
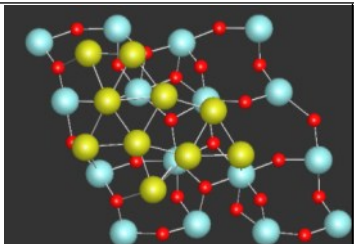
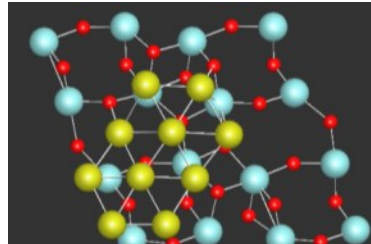
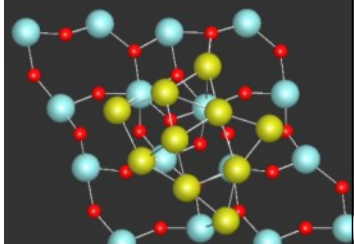
No.	Structure	E_{rel}	No.	Structure	E_{rel}
Au/ZrO_2					
1-1 (1)		0.00	1-3		0.37
1-2		0.002			
Au_2/ZrO_2					
2-1 (2)		0.00	2-3		0.35
2-2		0.14	2-4		2.02
Au_3/ZrO_2					
3-1 (3)		0.00	3-2		0.24
3-3		0.29	3-4		0.39
3-5		0.43	3-6		0.82
Au_4/ZrO_2					

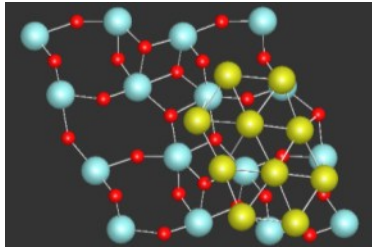
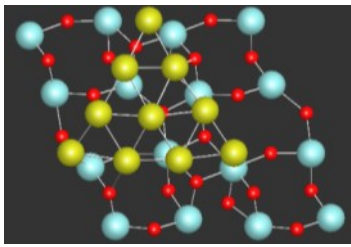
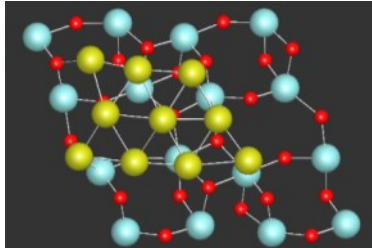
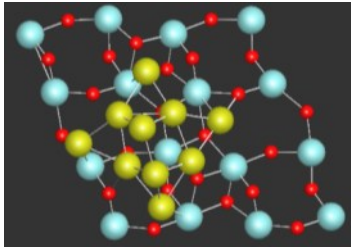
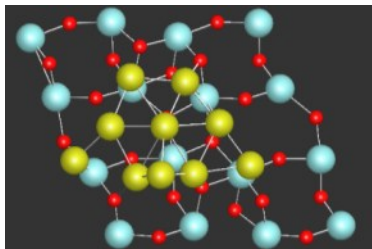
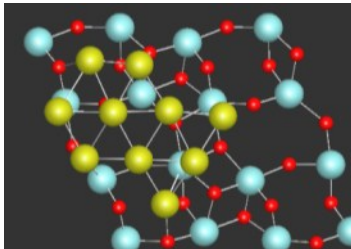
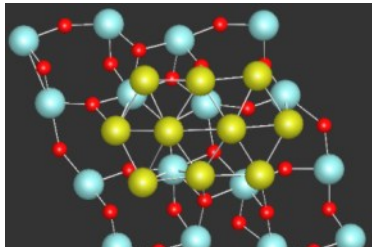
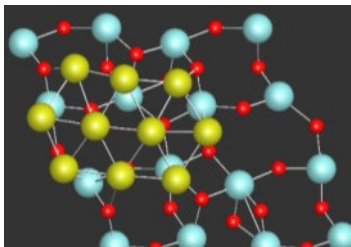
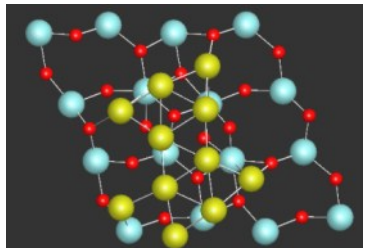
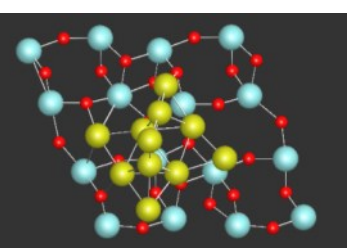
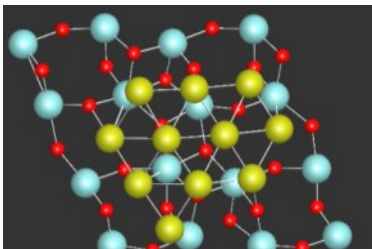
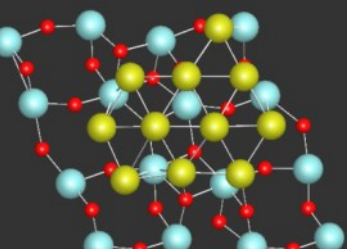
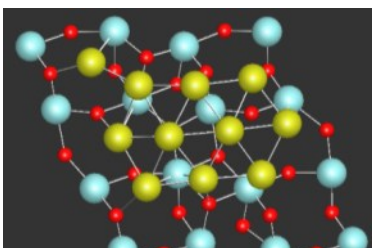
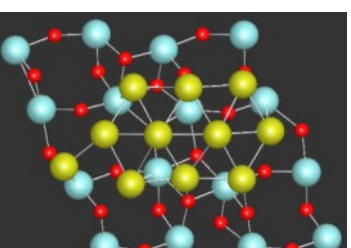
4-1 (4)		0.00	4-2		0.99
4-3		0.70	4-4		0.94
4-5		0.74	4-6		0.47
4-7		0.72	4-8		0.58
Au_5/ZrO_2					
5-1 (5)		0.00	5-2		0.19
5-3		0.20	5-4		0.44
5-5		0.37	5-6		0.55
5-7		0.62	5-8		0.36
5-9		0.01	5-10		0.04
5-11		0.05	5-12		0.43
Au_6/ZrO_2					

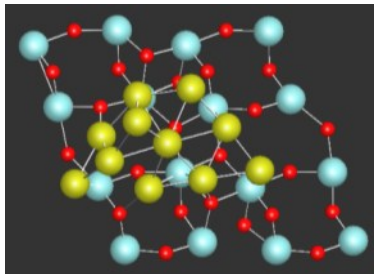
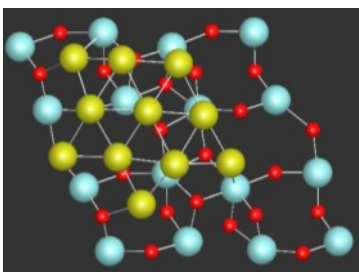
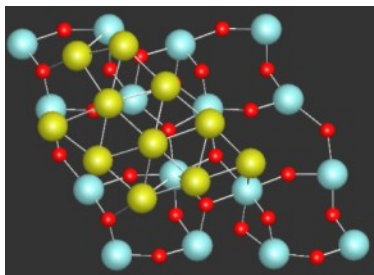
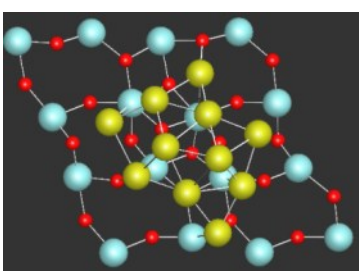
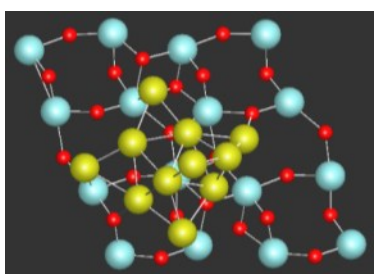
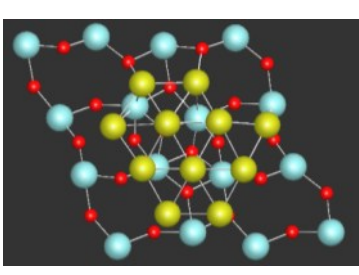
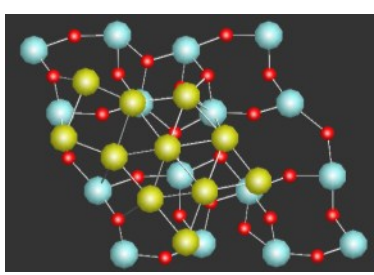
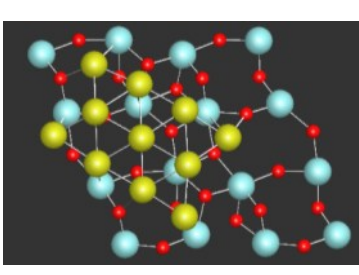
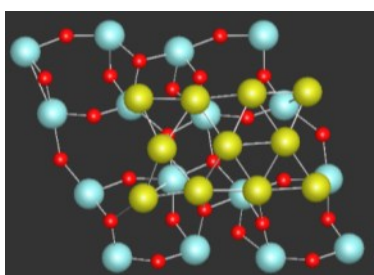
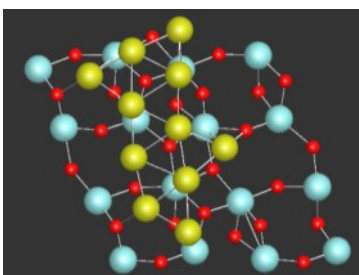
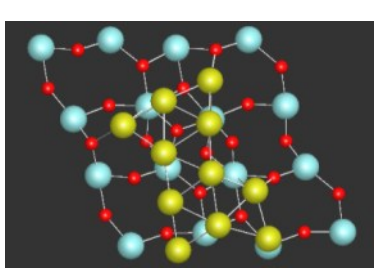
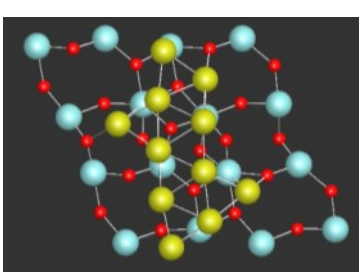
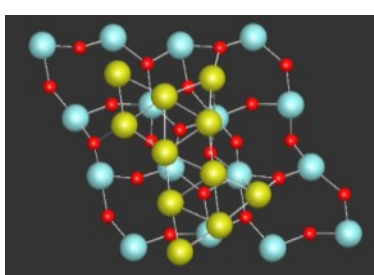
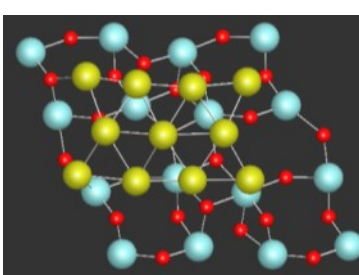
6-1 (6)		0.00	6-2		0.10
6-3		0.30	6-4		0.64
6-5		1.13	6-6		0.03
6-7		0.37	6-8		0.61
6-9		0.74			
Au_7/ZrO_2					
7-1 (7)		0.00	7-2		0.42
7-3		0.30	7-4		0.44
7-5		0.66	7-6		0.67
7-7		0.53	7-8		0.12
7-9		0.60	7-10		0.07

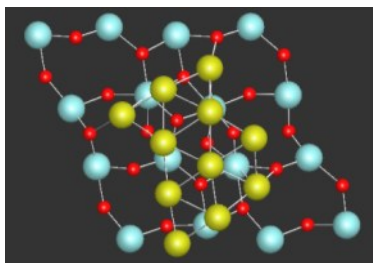
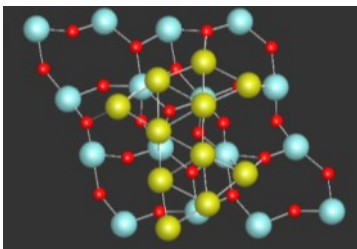
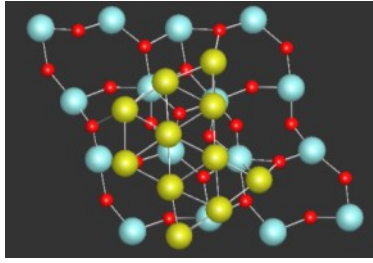
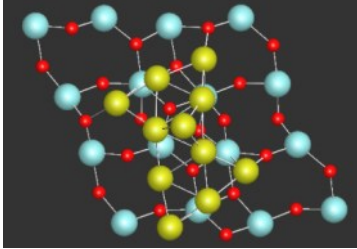
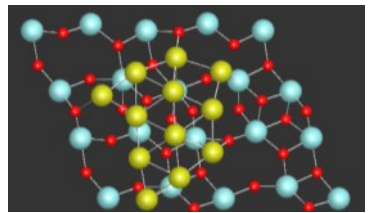
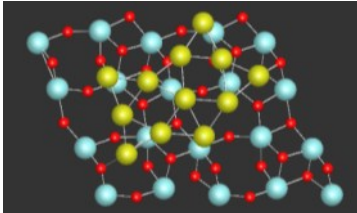
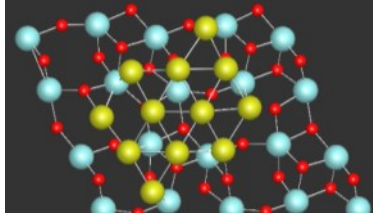
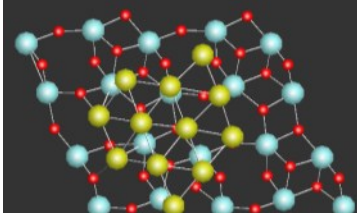
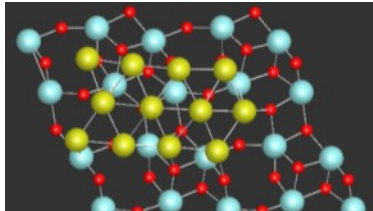
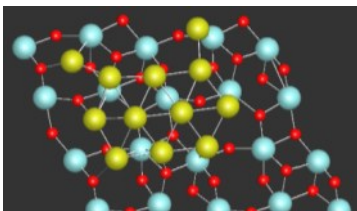
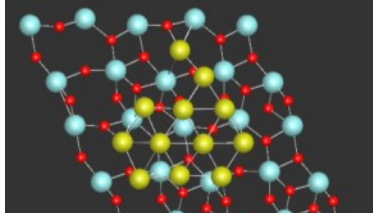
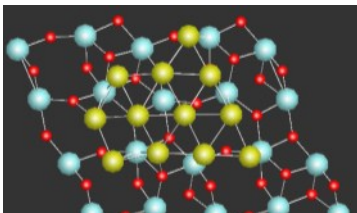
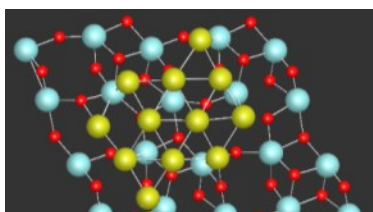
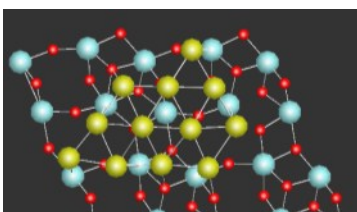
7-11		0.53	7-12		0.58
7-13		0.07	7-14		0.28
7-15		0.24			
Au_8/ZrO_2					
8-1 (8)		0.00	8-2		0.19
8-3		0.44	8-4		0.42
8-5		0.23	8-6		0.57
8-7		0.29	8-8		0.14
8-9		0.16	8-10		0.25

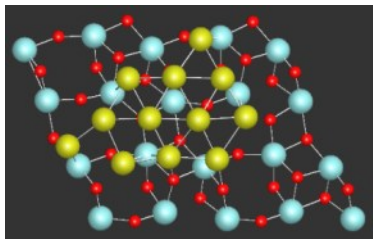
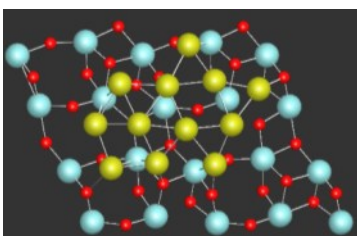
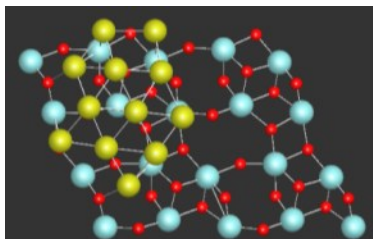
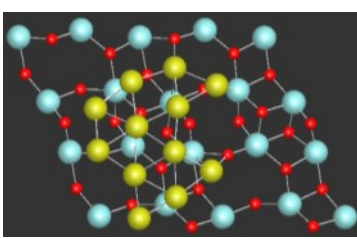
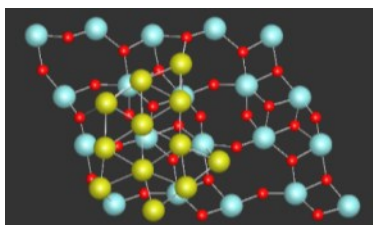
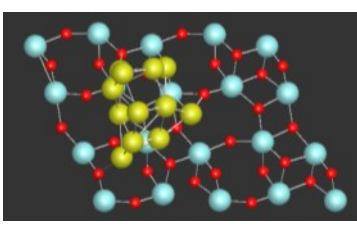
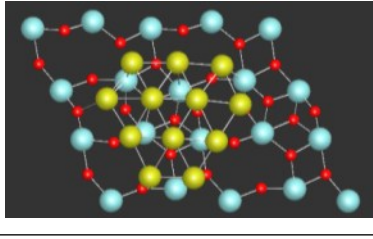
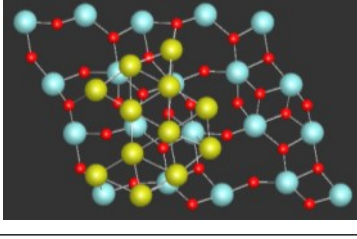
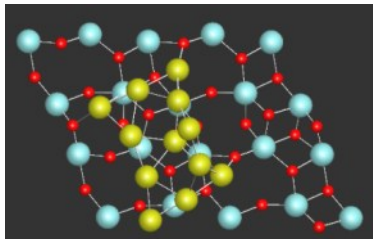
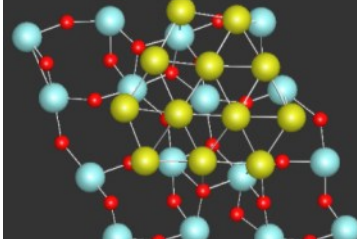
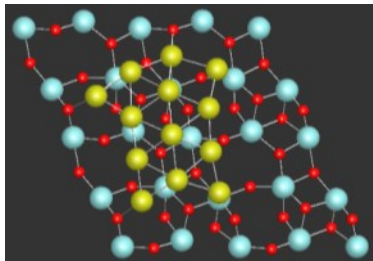
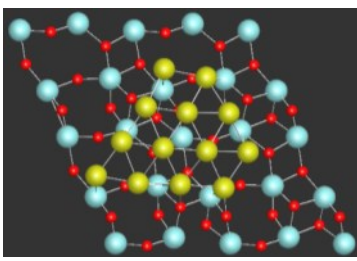
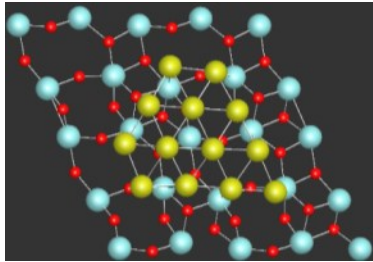
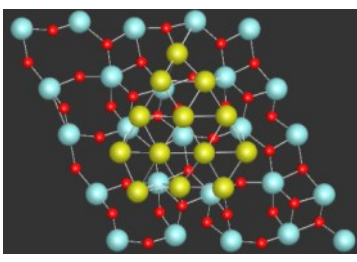
8-11		0.37	8-12		0.14
8-13		0.19	8-14		0.60
8-15		0.25	8-16		0.54
Au_9/ZrO_2					
9-1 (9)		0.00	9-2		0.89
9-3		0.66	9-4		0.66
9-5		0.47	9-6		0.73
9-7		0.59	9-8		1.16

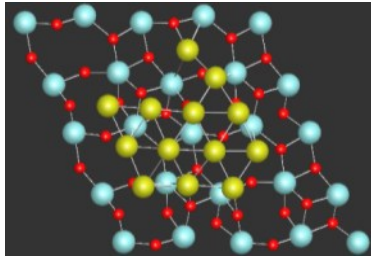
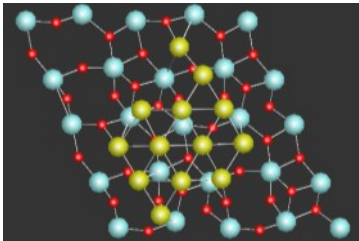
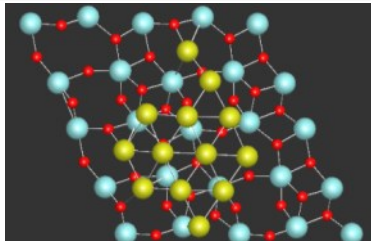
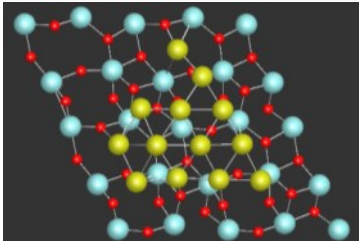
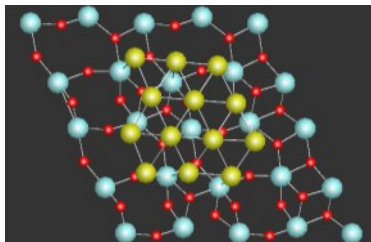
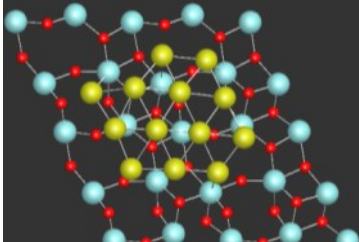
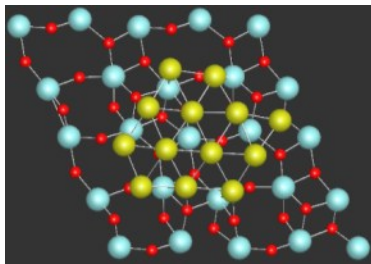
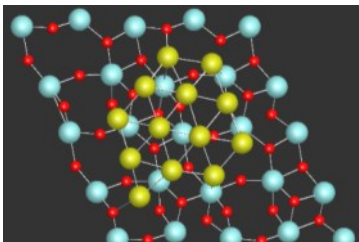
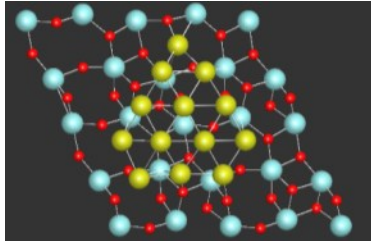
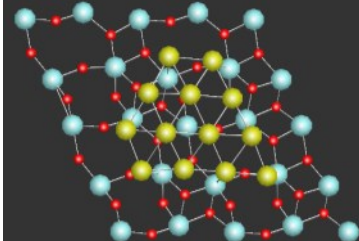
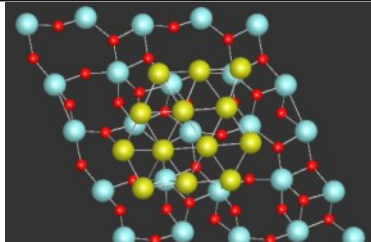
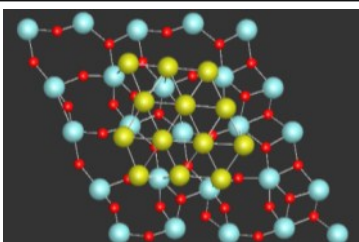
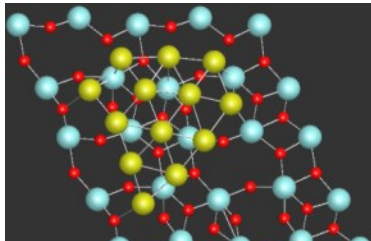
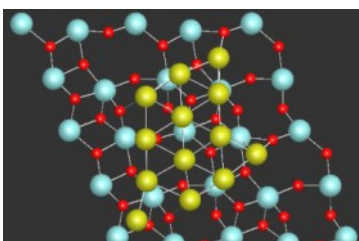
9-9		0.73	9-10		0.53
9-11		1.00	9-12		1.02
9-13		1.59	9-14		0.58
9-15		0.62	9-16		1.01
9-17		0.33			
$\text{Au}_{10}/\text{ZrO}_2$					
10-1 (10)		0.00	10-2		1.14
10-3		1.68	10-4		1.30

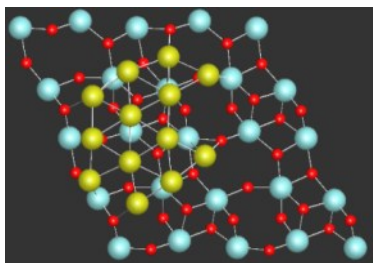
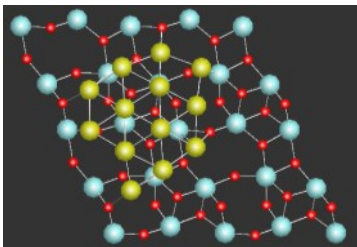
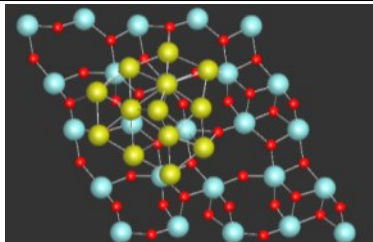
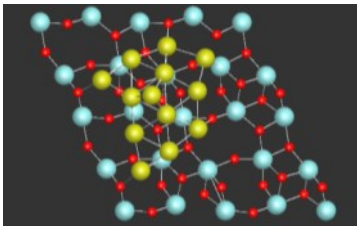
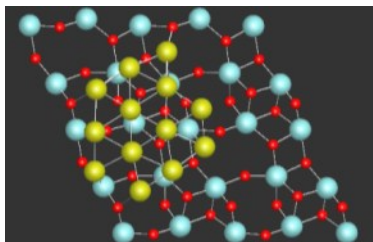
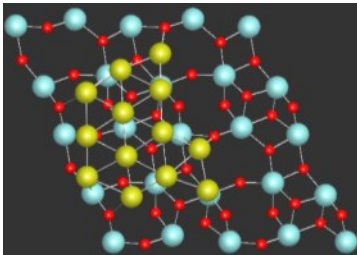
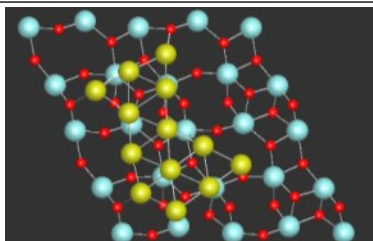
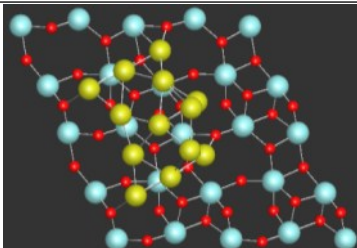
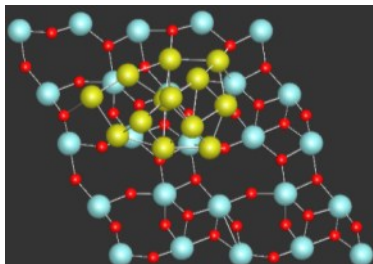
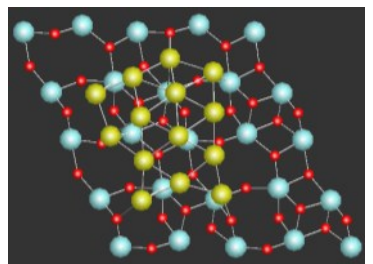
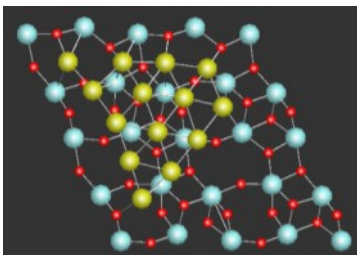
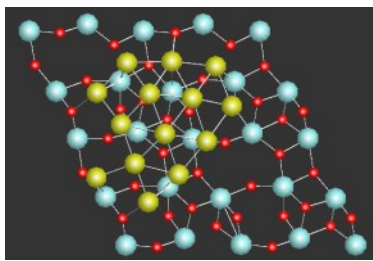
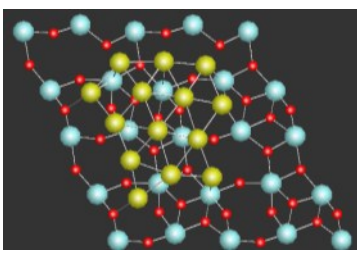
10-5		1.87	10-6		1.75
10-7		1.06	10-8		1.79
10-9		1.85	10-10		1.29
10-11		1.01	10-12		1.11
$\text{Au}_{11}/\text{ZrO}_2$					
11-1 (11)		0.00	11-2		1.64
11-3		1.00	11-4		0.74
11-5		1.11	11-6		0.94

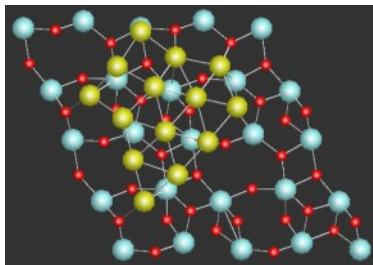
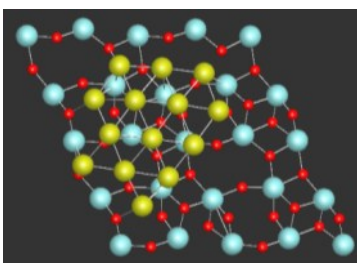
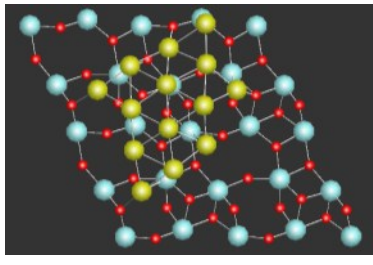
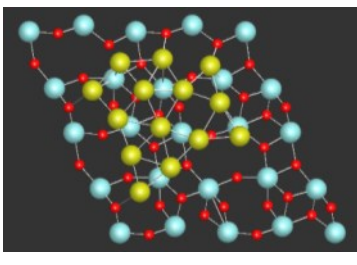
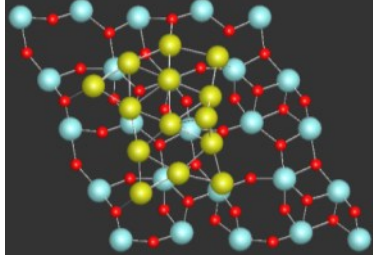
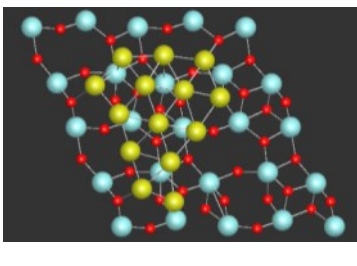
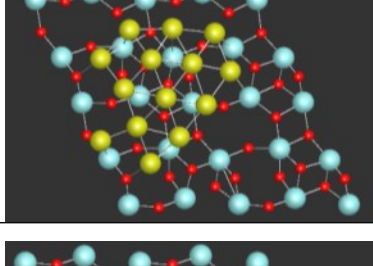
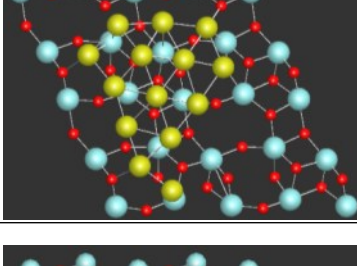
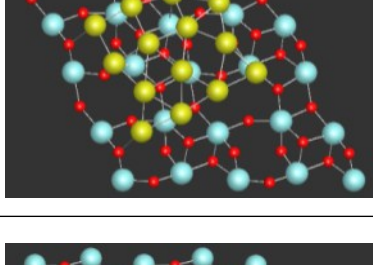
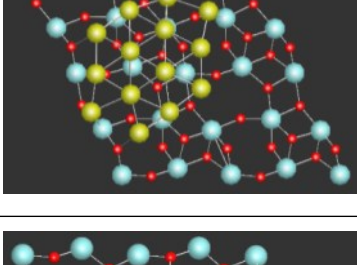
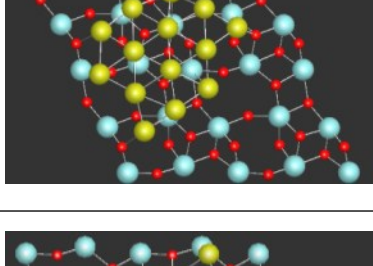
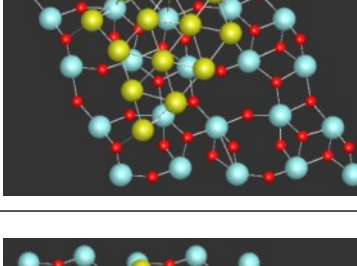
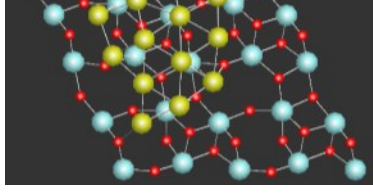
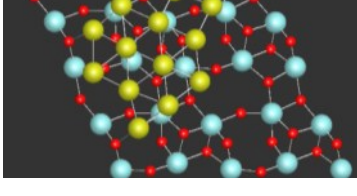
11-7		1.53	11-8		0.99
11-9		0.83	11-10		1.12
11-11		1.61	11-12		0.72
11-13		1.28	11-14		1.09
11-15		0.83	11-16		0.41
11-17		0.12	11-18		0.32
11-19		0.28	11-20		1.29

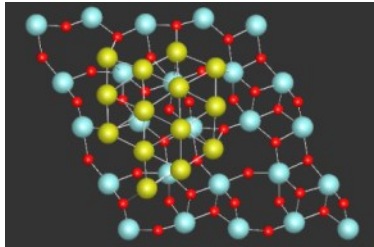
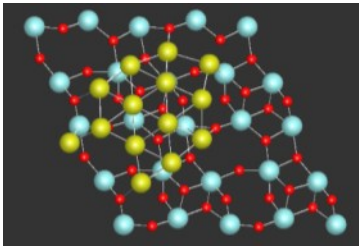
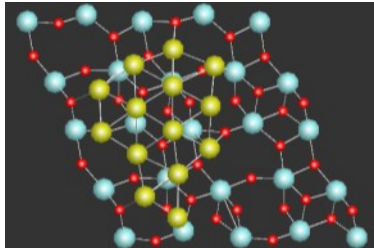
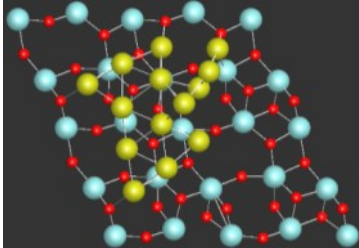
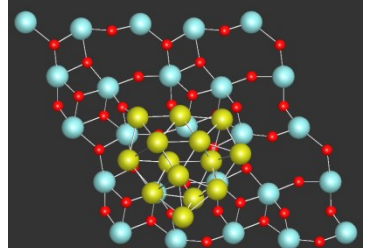
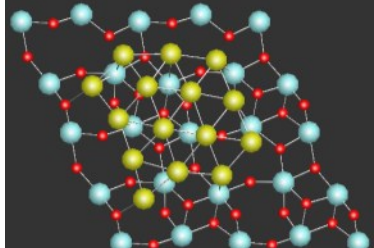
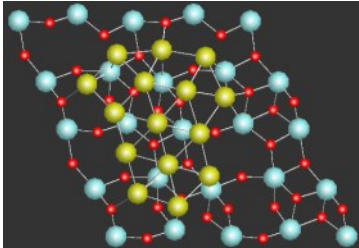
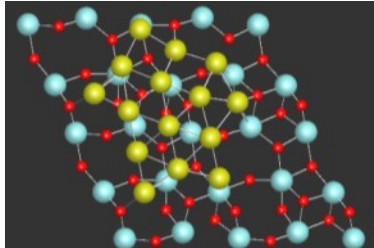
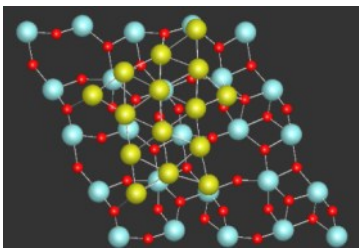
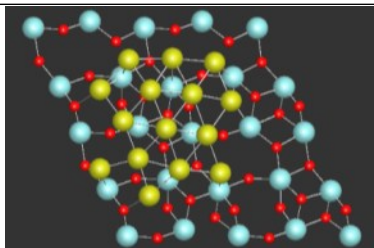
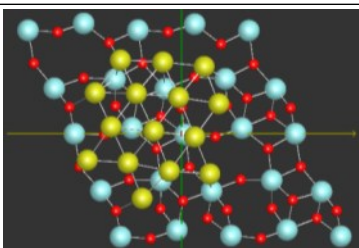
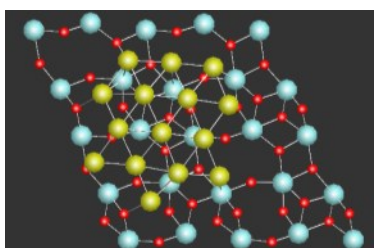
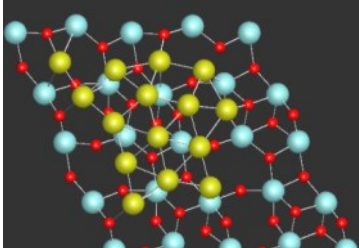
11-21		0.04	11-22		0.10
11-23		0.12	11-24		0.33
$\text{Au}_{12}/\text{ZrO}_2$					
12-1 (12)		0.00	12-2		0.91
12-3		1.45	12-4		1.29
12-5		1.66	12-6		1.38
12-7		0.63	12-8		0.95
12-9		1.46	12-10		1.37

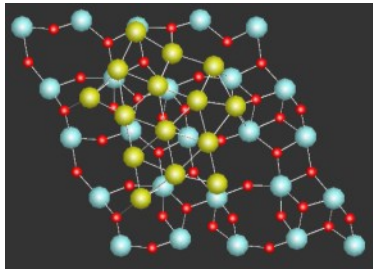
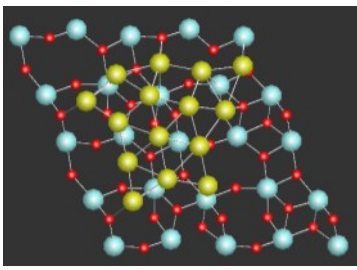
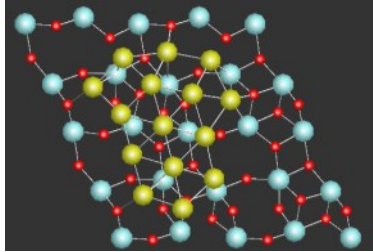
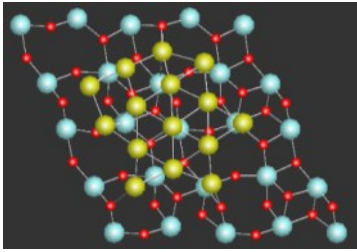
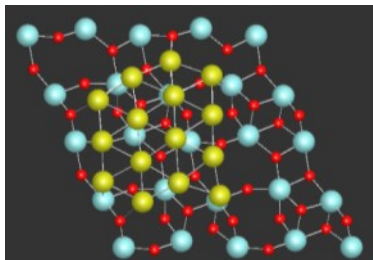
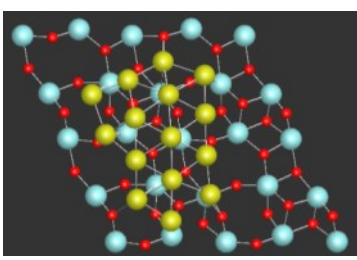
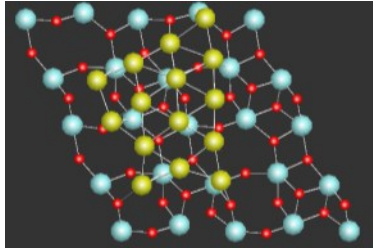
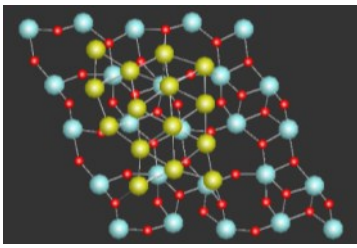
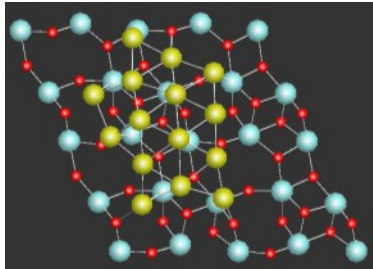
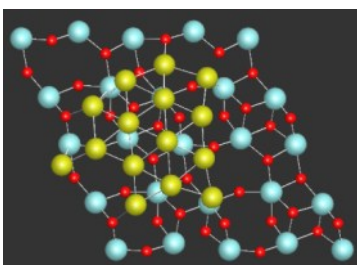
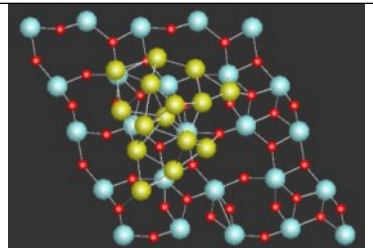
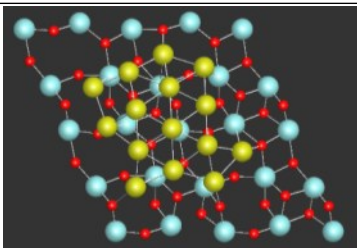
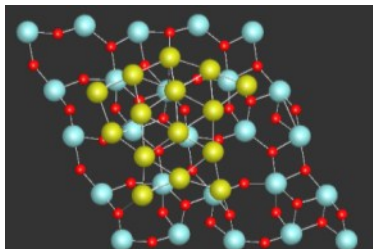
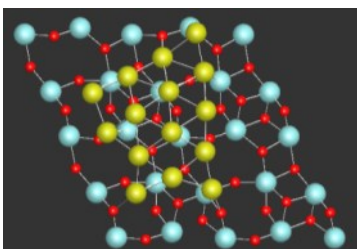
12-11		1.37	12-12		1.00
12-13		0.26	12-14		0.50
12-15		0.17	12-16		2.19
12-17		0.45	12-18		0.41
12-19		0.56	12-20		0.66
$\text{Au}_{13}/\text{ZrO}_2$					
13-1 (13)		0.00	13-2		0.77
13-3		0.72	13-4		0.45

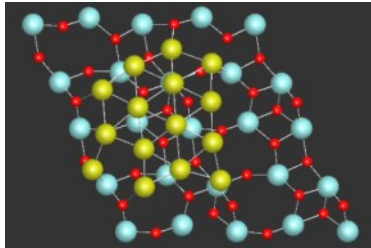
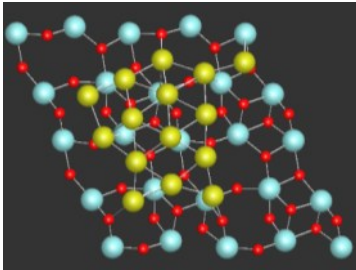
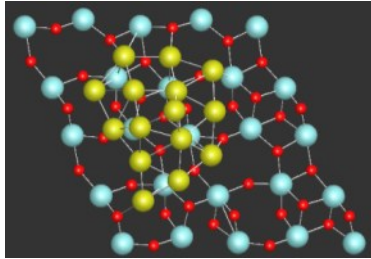
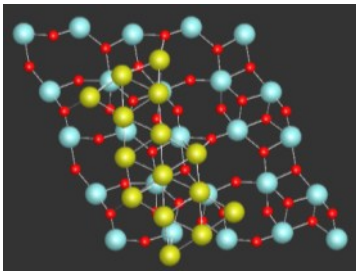
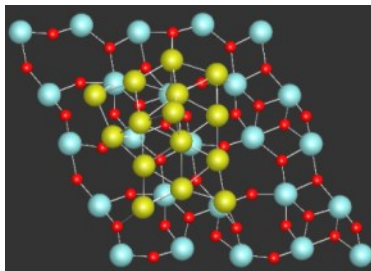
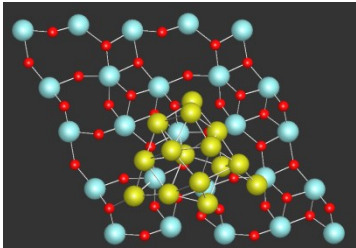
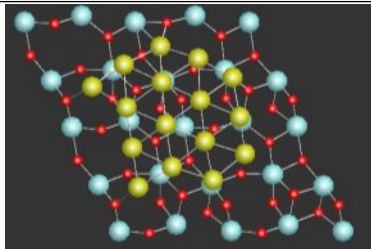
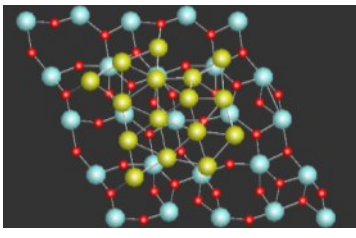
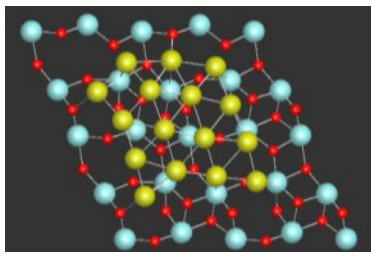
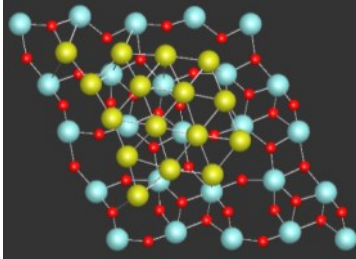
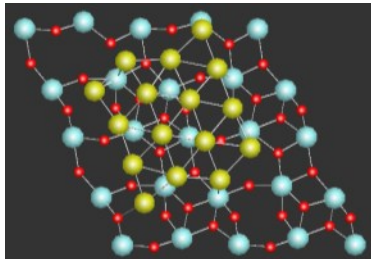
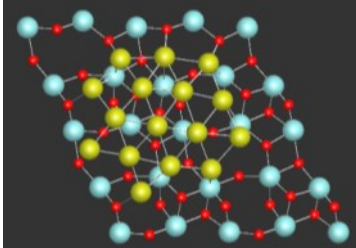
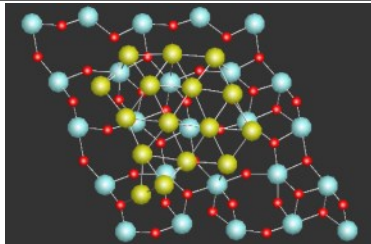
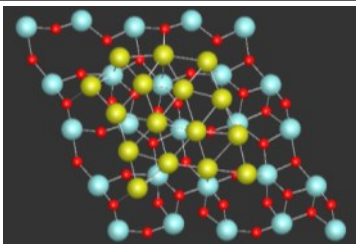
13-5		1.21	13-6		1.01
13-7		1.12	13-8		0.77
13-9		0.85	13-10		0.89
13-11		0.72	13-12		0.32
13-13		0.45	13-14		0.73
13-15		0.95	13-16		0.84
13-17		0.22	13-18		1.07

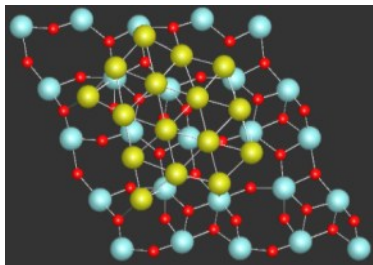
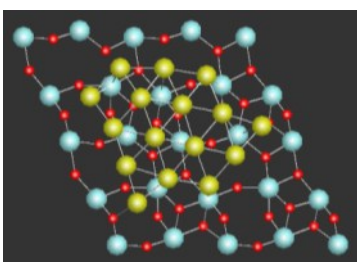
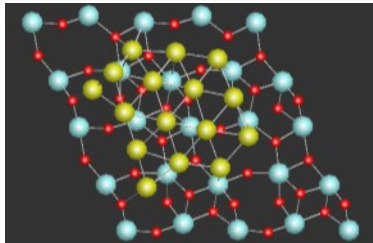
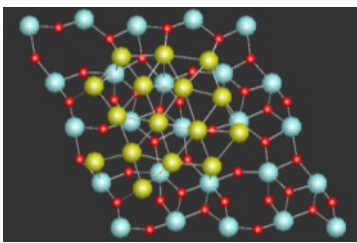
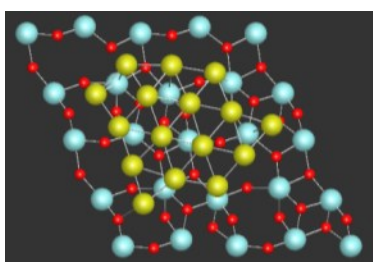
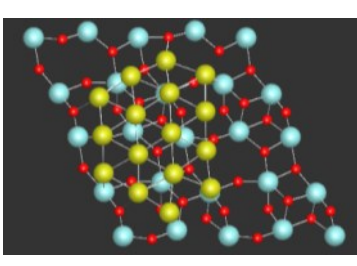
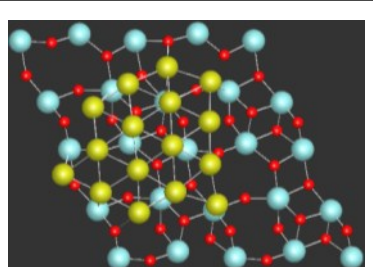
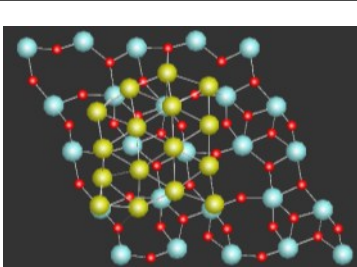
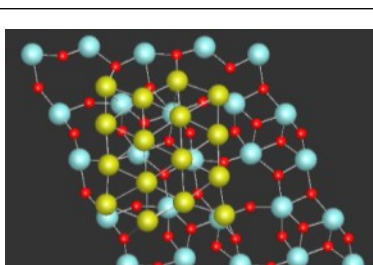
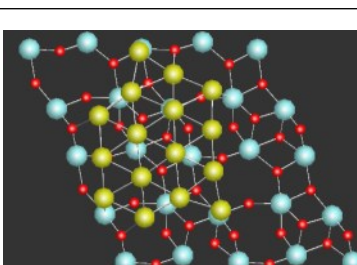
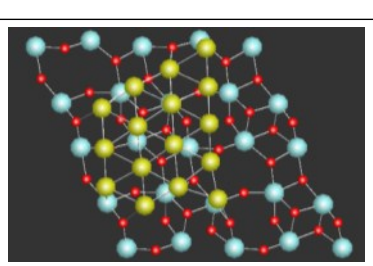
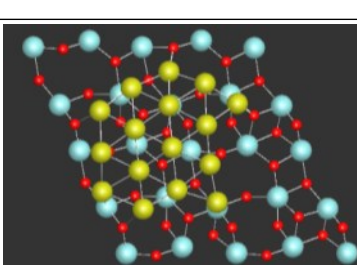
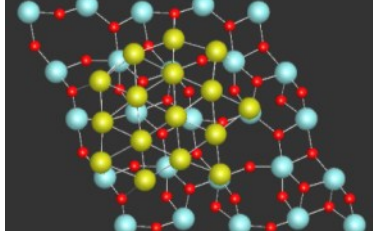
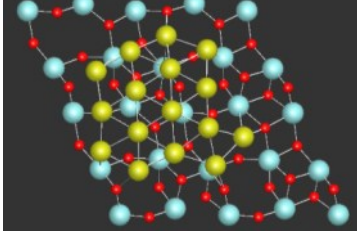
13-19		0.45	13-20		0.30
13-21		1.41	13-22		0.49
13-23		0.39	13-24		0.42
13-25		0.77	13-26		0.91
13-27		1.94			
$\text{Au}_{14}/\text{ZrO}_2$					
14-1 (14)		0.00	14-2		0.46
14-3		0.30	14-4		0.12

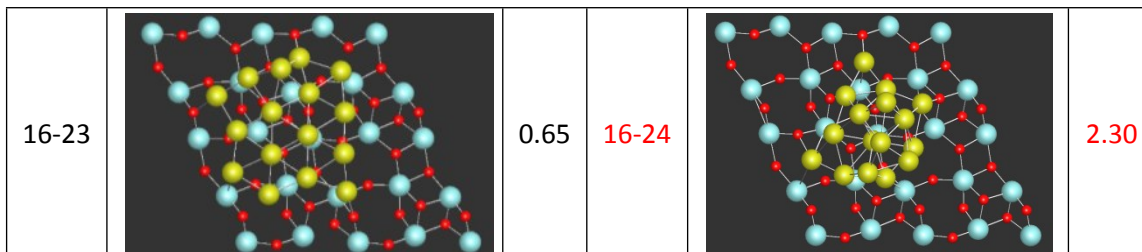
14-5		0.44	14-6		0.17
14-7		0.15	14-8		0.16
14-9		0.20	14-10		0.84
14-11		0.31	14-12		0.91
14-13		0.31	14-14		0.22
14-15		0.39	14-16		0.68
14-17		0.72	14-18		0.71

14-19		0.38	14-20		0.45
14-21		1.18	14-22		0.43
14-23		1.89			
$\text{Au}_{15}/\text{ZrO}_2$					
15-1 (15)		0.00	15-2		0.79
15-3		0.30	15-4		0.35
15-5		0.21	15-6		0.17
15-7		0.16	15-8		0.36

15-9		0.30	15-10		0.65
15-11		0.78	15-12		0.09
15-13		0.09	15-14		0.82
15-15		0.70	15-16		0.65
15-17		0.56	15-18		0.37
15-19		1.66	15-20		0.21
15-21		0.61	15-22		0.70

15-23		0.21	15-24		0.62
15-25		0.86	15-26		1.34
15-27		0.58	15-28		2.07
$\text{Au}_{16}/\text{ZrO}_2$					
16-1 (16)		0.00	16-2		0.15
16-3		0.14	16-4		0.53
16-5		0.73	16-6		0.48
16-7		0.88	16-8		0.13

16-9		0.40	16-10		0.15
16-11		0.42	16-12		0.58
16-13		0.14	16-14		0.91
16-15		0.20	16-16		0.69
16-17		0.31	16-18		0.71
16-19		0.89	16-20		0.31
16-21		0.43	16-22		0.50



3. The detailed charge distributions for $\text{Au}_{10}/\text{ZrO}_2$ and $\text{Au}_{16}/\text{ZrO}_2$

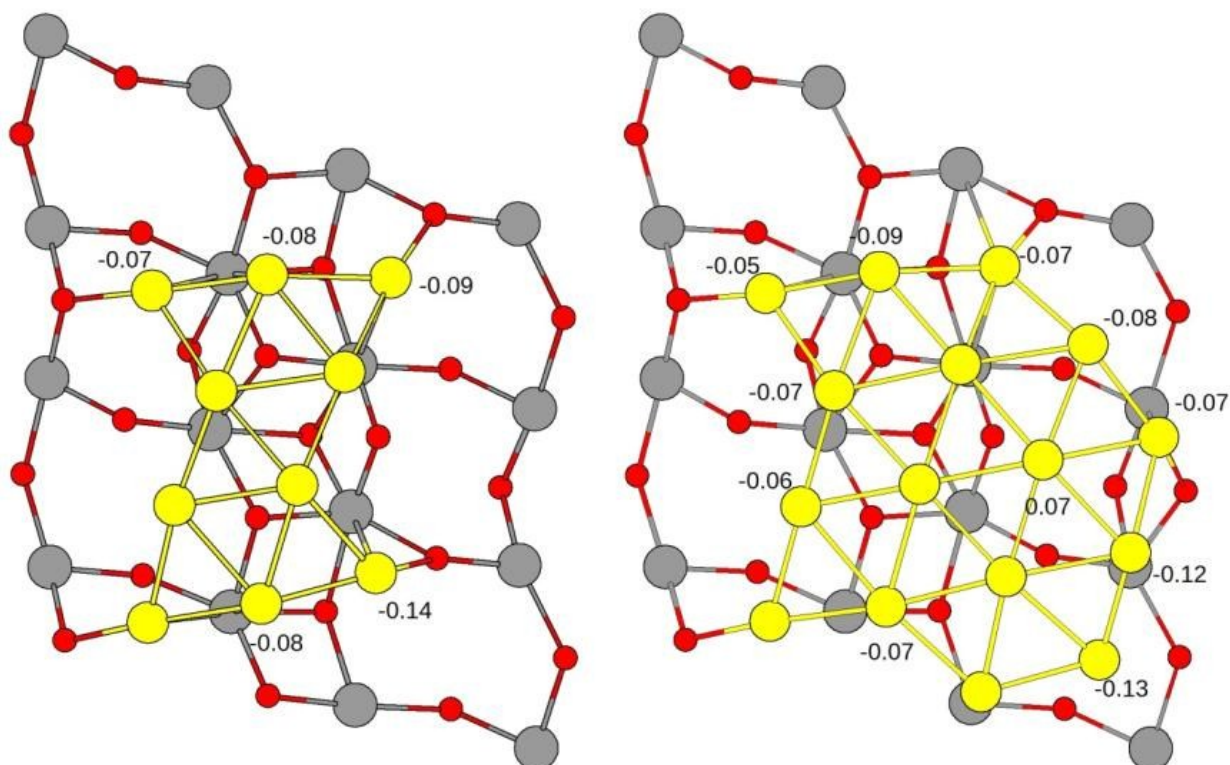


Figure S1 The charge distributions on the Au atoms in $\text{Au}_{10}/\text{ZrO}_2$ and $\text{Au}_{16}/\text{ZrO}_2$. (Only the net charges being beyond 0.05e were marked.), It is clear that the charge transfer from ZrO_2 surface to the Au atoms mainly occurs on the Au atoms in the perimeter region of the Au_n cluster.

4. The HOMO of the Au_n/ZrO_2

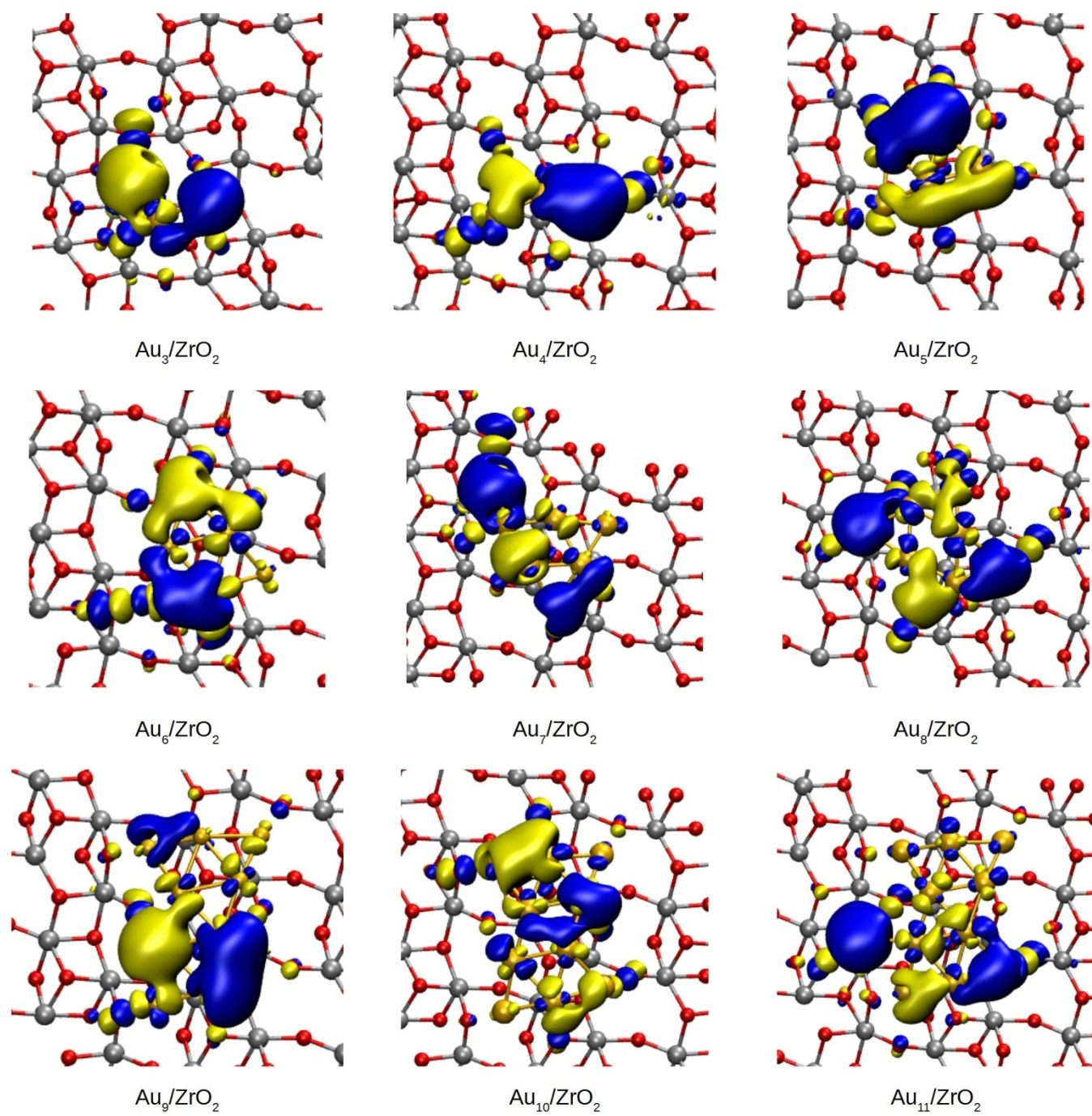


Figure S2 The HOMO of Au_n/ZrO_2 ($n=3-11$).

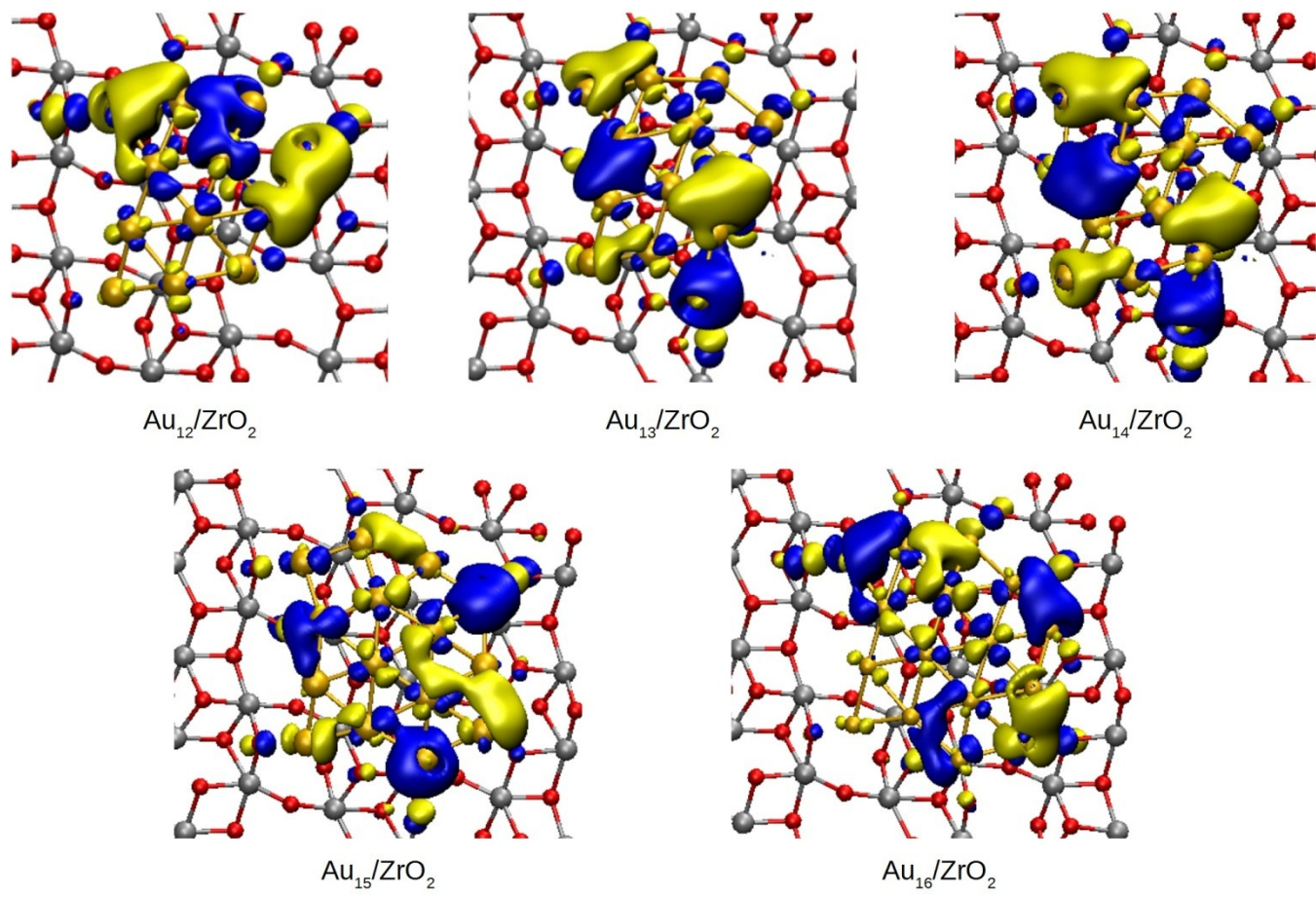


Figure S3 The HOMOs of Au_n/ZrO_2 ($n=12-16$)