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

Structural and Electronic properties of Au_n clusters on α-Al_2O_3(0001) surface: A first principles study

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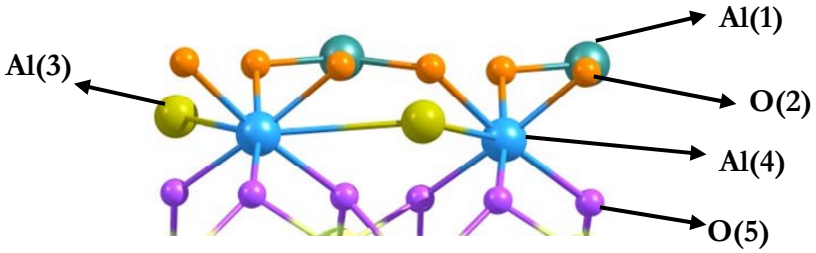
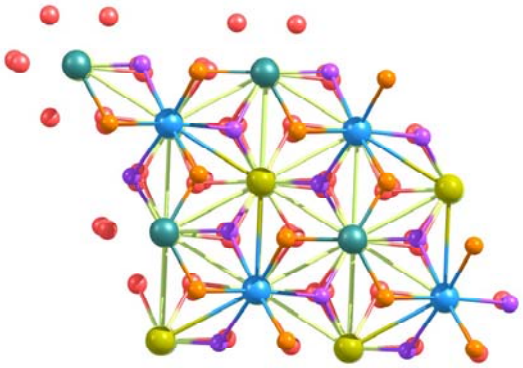
Supporting information

Figure S1: Side and Top views of Al_2O_3 surface.



(a) Side View of top five layers of α-Al_2O_3(0001) surface



(b) Top View of α-Al_2O_3(0001) surface

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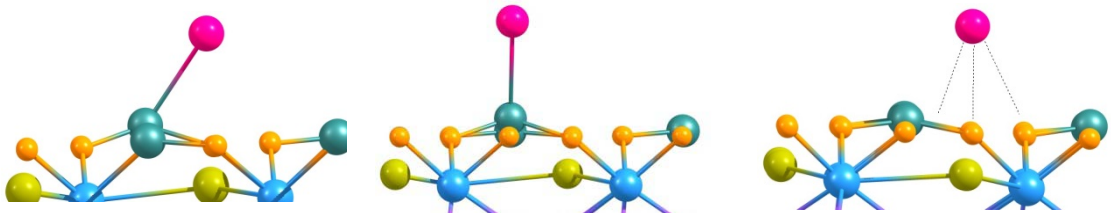
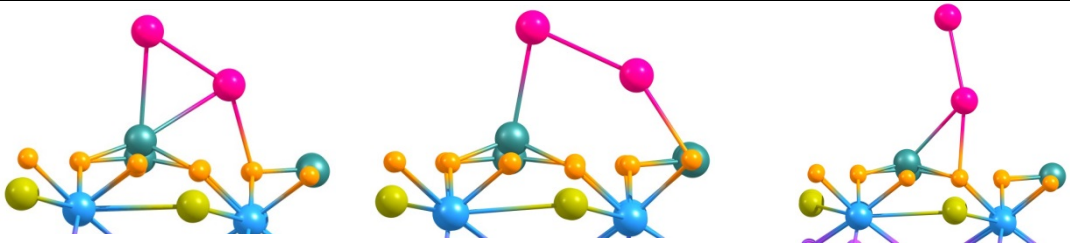
Figure S2: Side views of low lying configurations of the Au_n clusters deposited on α-Al_2O_3(0001) surface.



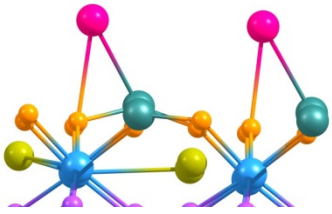
Au$_1$

ΔE=0.00 **ΔE=0.09** **ΔE=0.47**

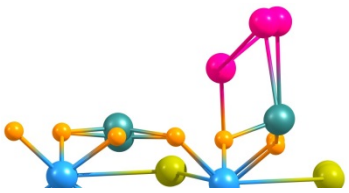
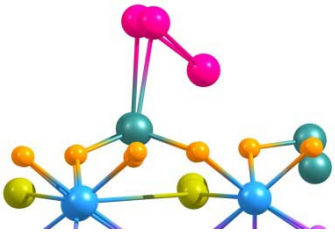
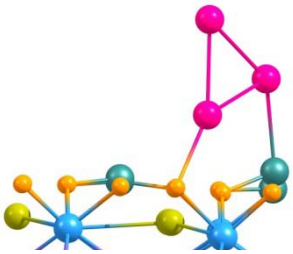
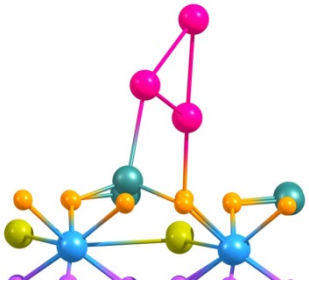
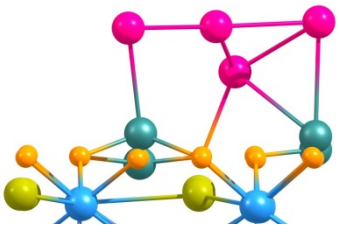
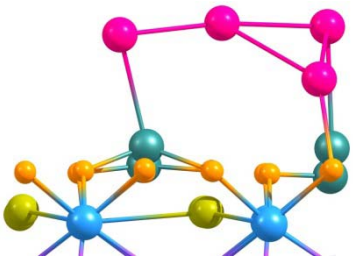
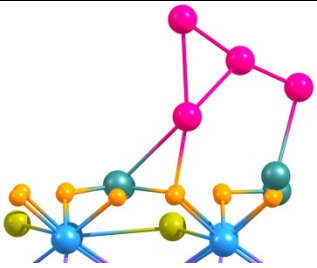


Au$_2$

ΔE=0.00 **ΔE=0.14** **ΔE=0.25**



ΔE=2.16

Au_3			
	ΔE=0.00	**ΔE=0.25**	**ΔE=0.32**
			
	ΔE=0.46		
Au_4			
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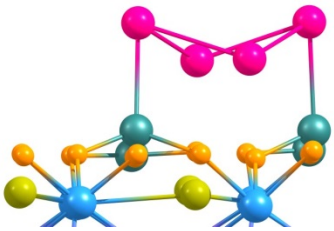
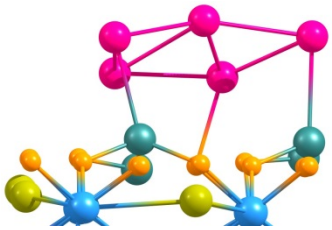
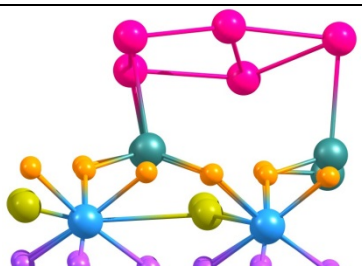
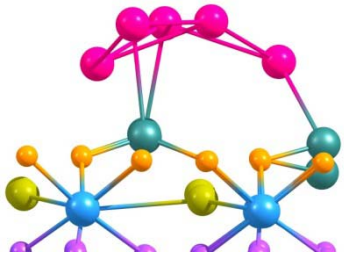
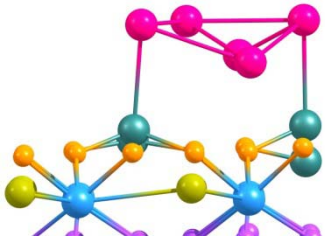
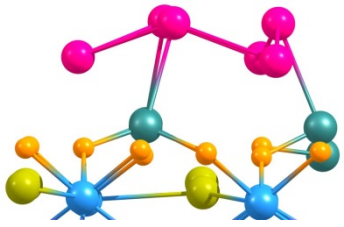
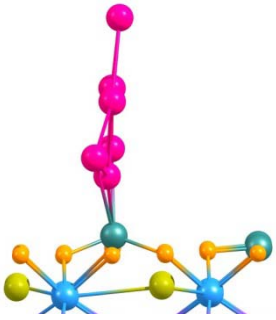
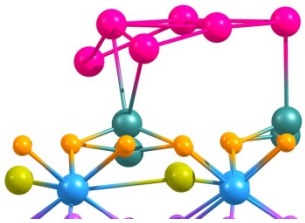
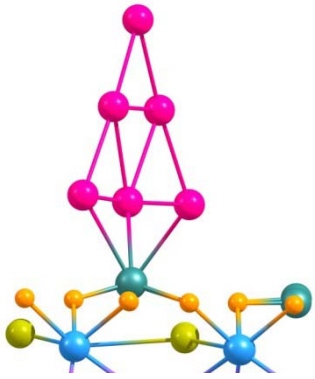
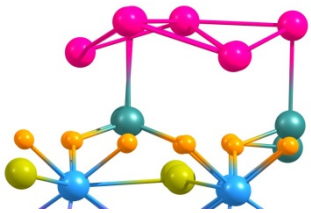
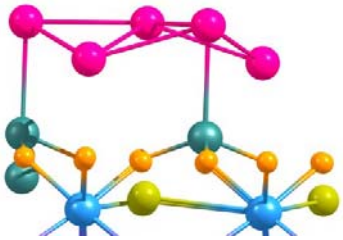
			
	ΔE=0.40		

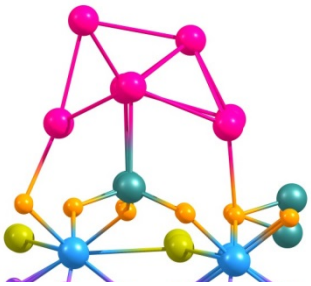
Au_5			
	ΔE=0.00	**ΔE=0.15**	**ΔE=0.17**
			
	ΔE=0.26		
Au_6			
	ΔE=0.00	**ΔE=0.43**	**ΔE=0.55**
			
	ΔE=0.69		



ΔE=0.00

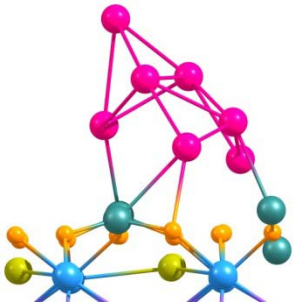


ΔE=0.44 (mb=1)

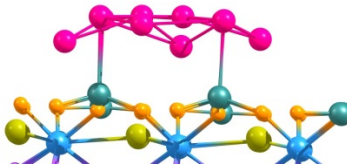


ΔE=0.44

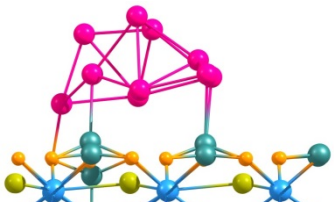
Au_7



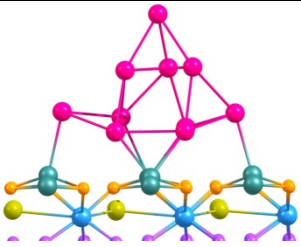
ΔE=0.47



ΔE=0.00

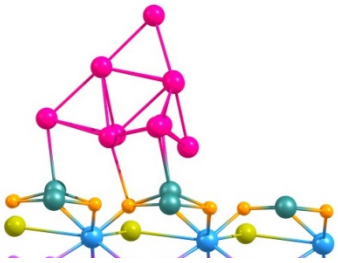


ΔE=0.28

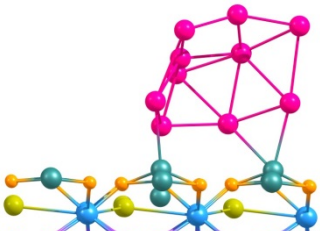


ΔE=0.47

Au_{10}

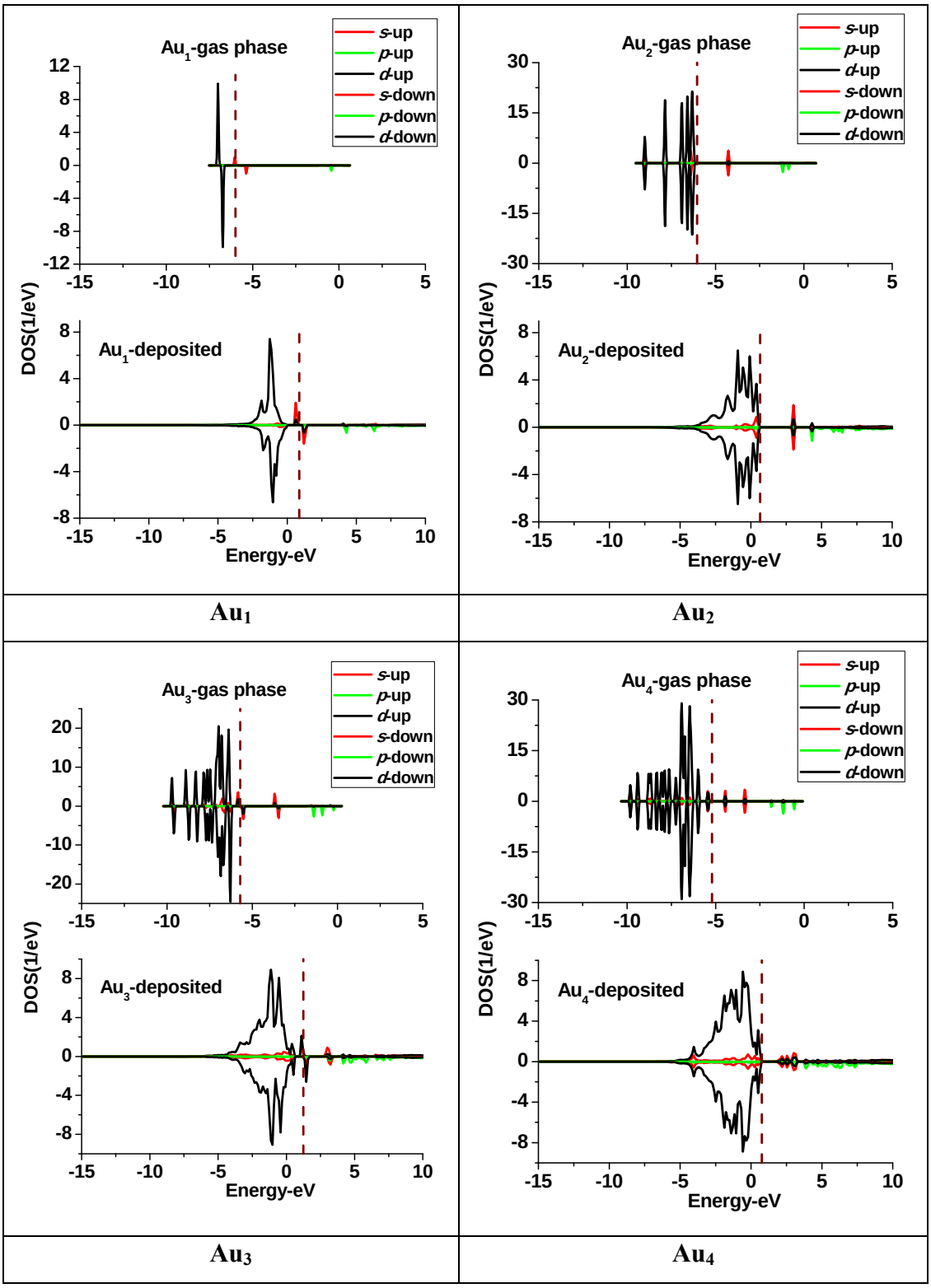


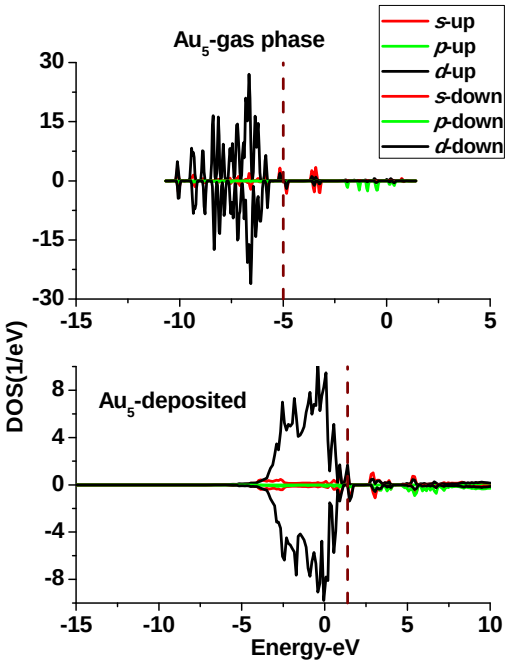
ΔE=0.97



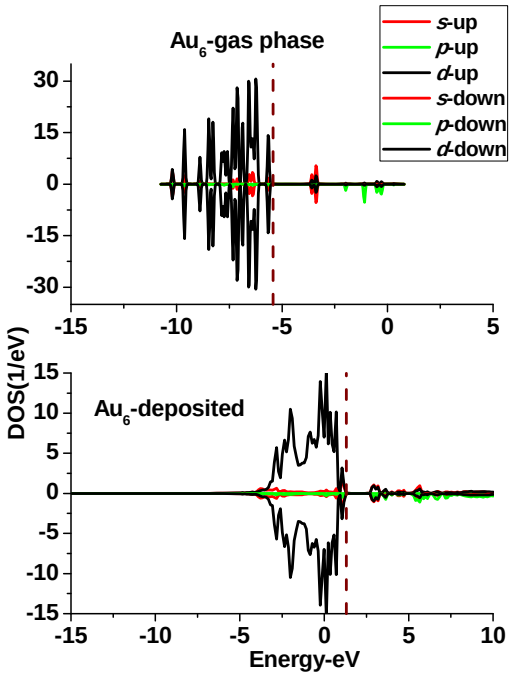
ΔE=1.06

Figure-S3: Comparison of the density of the states (PDOS) plot.

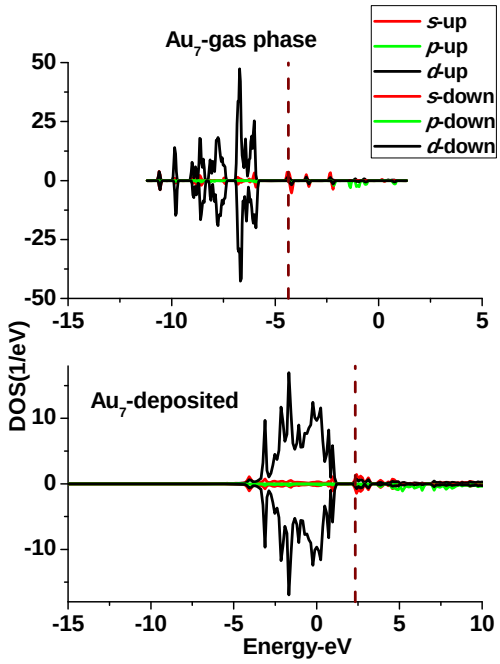




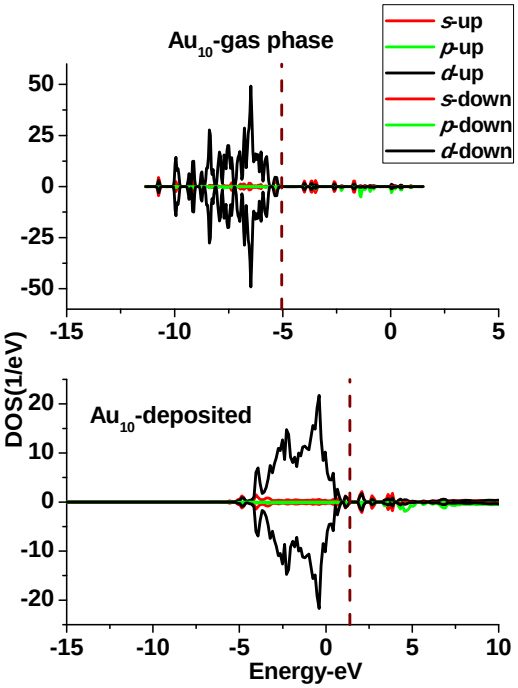
Au_5



Au_6



Au_7



Au_{10}