Electronic Supplementary Information for

Probing electronic structure of Co_n (n = 1-5) clusters on γ-Al_2O_3 surfaces by first-principle calculations

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Content

I. The Co-Co bond distances of Co_n (n = 2-5) clusters in the gas phase and on the dehydrated (100) and hydrated (110) surfaces.

Table S1. The Co-Co bond distances of Co_n (n = 2-5) clusters in the gas phase and on the dehydrated (100) and hydrated (110) surfaces.

Cluster		Bond distances								
2	gas phase	1.956								
	dehydrated (100)	2.089								
	hydrated (110)	2.036								
3	gas phase	2.049	2.089	2.504						
	dehydrated (100)	2.264	2.079	2.418						
	hydrated (110)	2.14	2.108	2.291						
4	gas phase	2.133	2.13	2.714	2.719	2.135	2.130			
	dehydrated (100)	2.15	2.193	2.608	2.238	2.113	2.457			
	hydrated (110)	2.142	2.151	2.547	2.273	2.304	2.496			
5	gas phase	2.179	2.18	2.642	2.644	2.641	2.179	2.181	2.18	2.179
	dehydrated (100)	2.162	2.577	2.19	2.29	2.357	2.345	2.416	2.089	2.675
	hydrated (110)	2.273	2.294	2.187	2.287	2.307	2.591	2.171	2.154	2.526

II. Electron density difference map of Co_n (n = 1, 2, 4, and 5) on the dehydrated (100) and hydrated (110) surfaces.

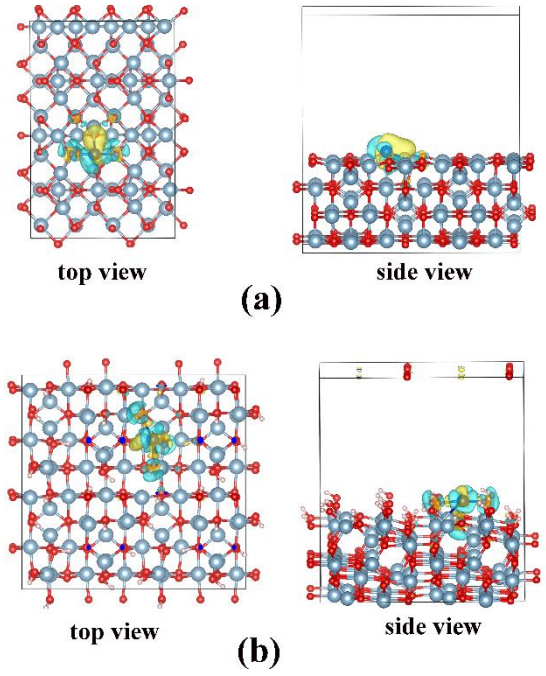

Fig. S1 Electron density difference map (isovalue = 0.04) for Co_1 cluster adsorbed on the (a)

dehydrated γ-Al_2O_3(100) surface and (b) hydrated γ-Al_2O_3(110) surface.

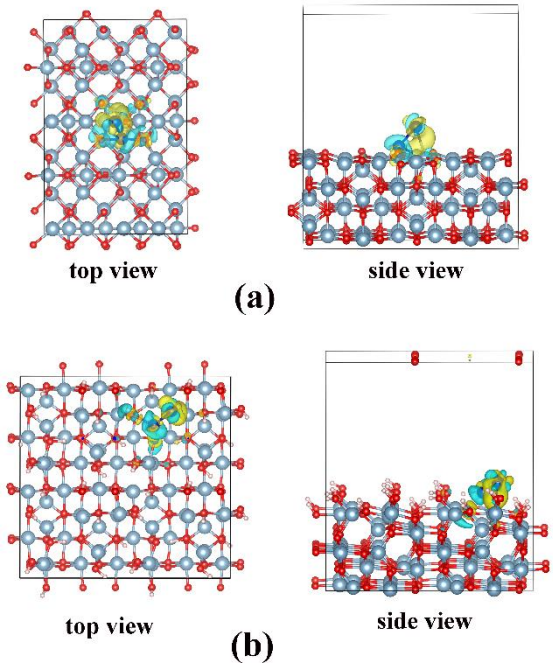

Fig. S2 Electron density difference map (isovalue = 0.04) for Co_2 cluster adsorbed on the (a) dehydrated γ-Al_2O_3(100) surface and (b) hydrated γ-Al_2O_3(110) surface.

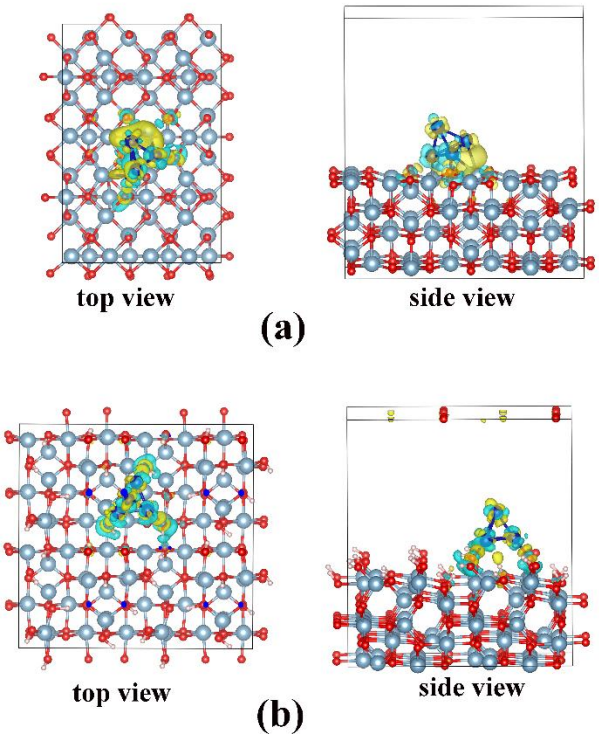

Fig. S3 Electron density difference map (isovalue = 0.04) for Co_4 cluster adsorbed on the (a) dehydrated γ-Al_2O_3(100) surface and (b) hydrated γ-Al_2O_3(110) surface.

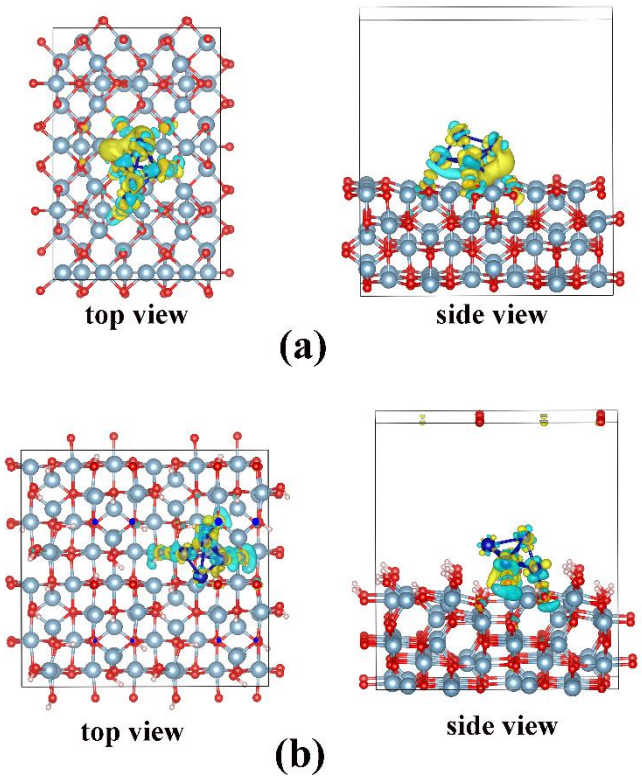

Fig. S4 Electron density difference map (isovalue = 0.04) for Co_5 cluster adsorbed on the (a) dehydrated γ-Al_2O_3(100) surface and (b) hydrated γ-Al_2O_3(110) surface.