Supporting Information

Adsorption of an Au atom and dimer on thin film θ-Al_2O_3/NiAl(100): dependence on the thickness of thin film θ-Al_2O_3

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Fig. S1 compares the DOS of Al in the top layer of bulk θ-Al_2O_3 (upper) and the monolayer alumina in model ***1L*** (lower). The former shows obviously a band gap between HOMO and LUMO, reflecting a feature of insulators; in contrast, the latter shows no band gap — clear DOS exists between energy 2.5 eV and -2.5 eV. The monolayer alumina supported on NiAl(100) has thus a fingerprint of metallic band structures.

Some meta-stable configurations without high symmetry are also found for an Au_2 dimer. Fig. S2(a) exemplifies a meta-stable configuration appearing in models ***1L***, ***2L***-O-Al, ***4L***, and ***5L***-O-Al, with $E_{Au_2}^{ads}$ = 0.3 ~ 0.6 eV. The Au dimer is standing at site No.9 and tilting toward site No.3, with a tilting angle 30° relative to the surface normal. Fig. S2(b) shows a meta-stable configuration found in models ***1L*** and ***4L***. The Au dimer is lying flat on the surface with small $E_{Au_2}^{ads}$ = 0.3 ~ 0.9 eV; one Au is located at site No.3 and the other at site No.11. Fig. S2(c) shows a meta-stable configuration appearing only in model ***1L***, with $E_{Au_2}^{ads}$ = 0.7 eV. The Au dimer is lying flat on the surface; one of them is bound to the Al atom (on site No.3) and the other located at site No.9.

Figure S1

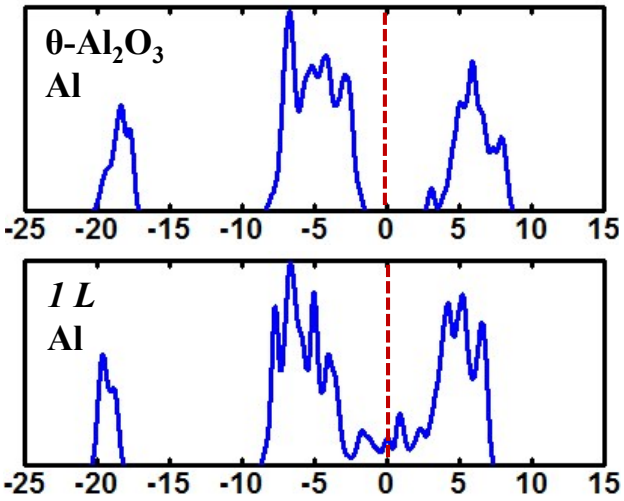

Fig. S1 Calculated DOS for Al in (a) the top layer of bulk θ-Al_2O_3(001) and (b) the monolayer alumina in ***1L*** θ-Al_2O_3/NiAl(100) (model ***1L***), as indicated. The dashed line

in the figure indicate the Fermi energy.

Figure S2

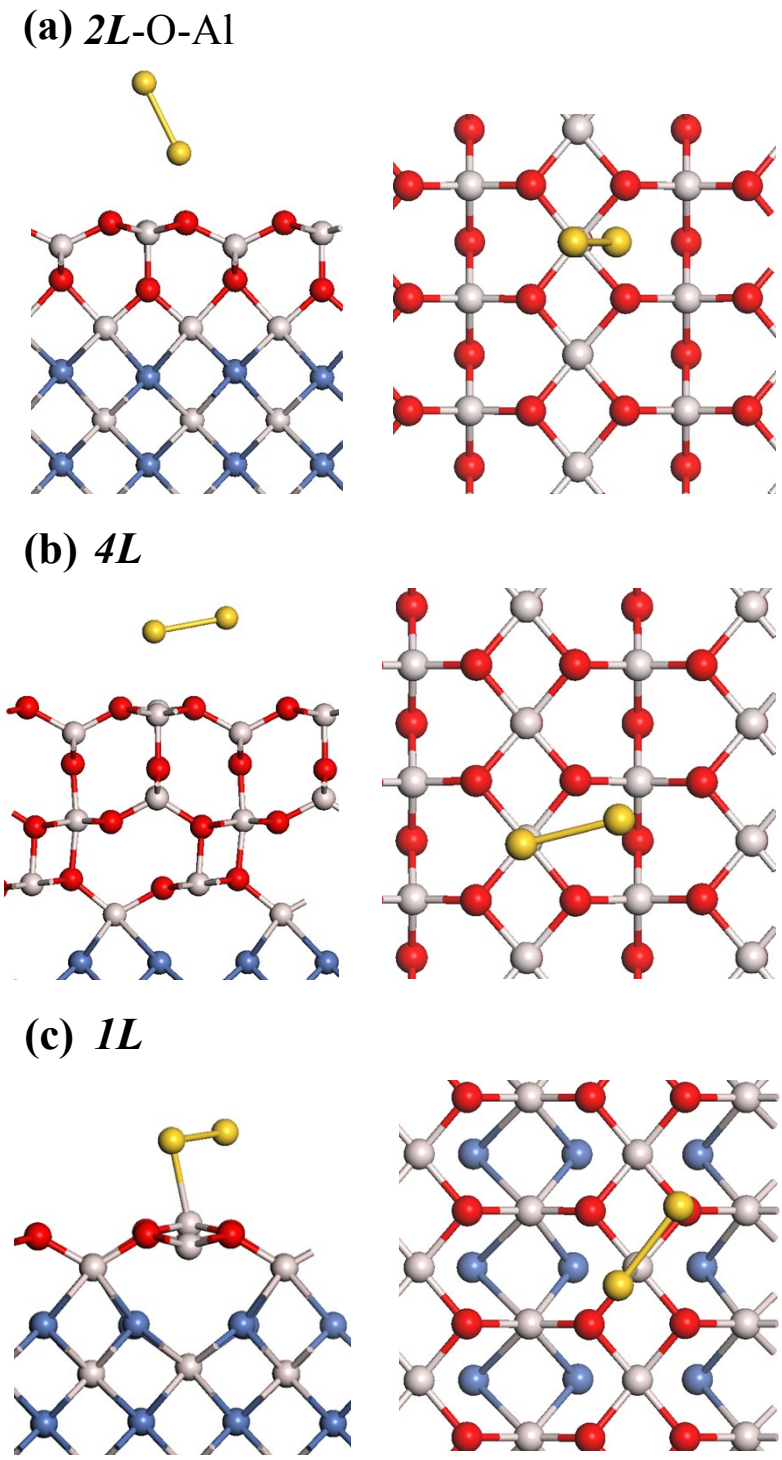

Fig. S2 Schematic diagrams showing side (left) and top views (right) for an Au dimer

adsorbed in a meta-stable configuration on θ-Al_2O_3/NiAl(100) surfaces in models (a) ***2L***-O-Al, (b) ***4L*** and (c) ***1L***. Red, grey and blue spheres denote O, Al and Ni atoms, respectively; yellow spheres denote adsorbed Au dimers.