Supporting Information

Wurtzite AlN(0001) Surface Oxidation: Hints from Ab Initio Calculations

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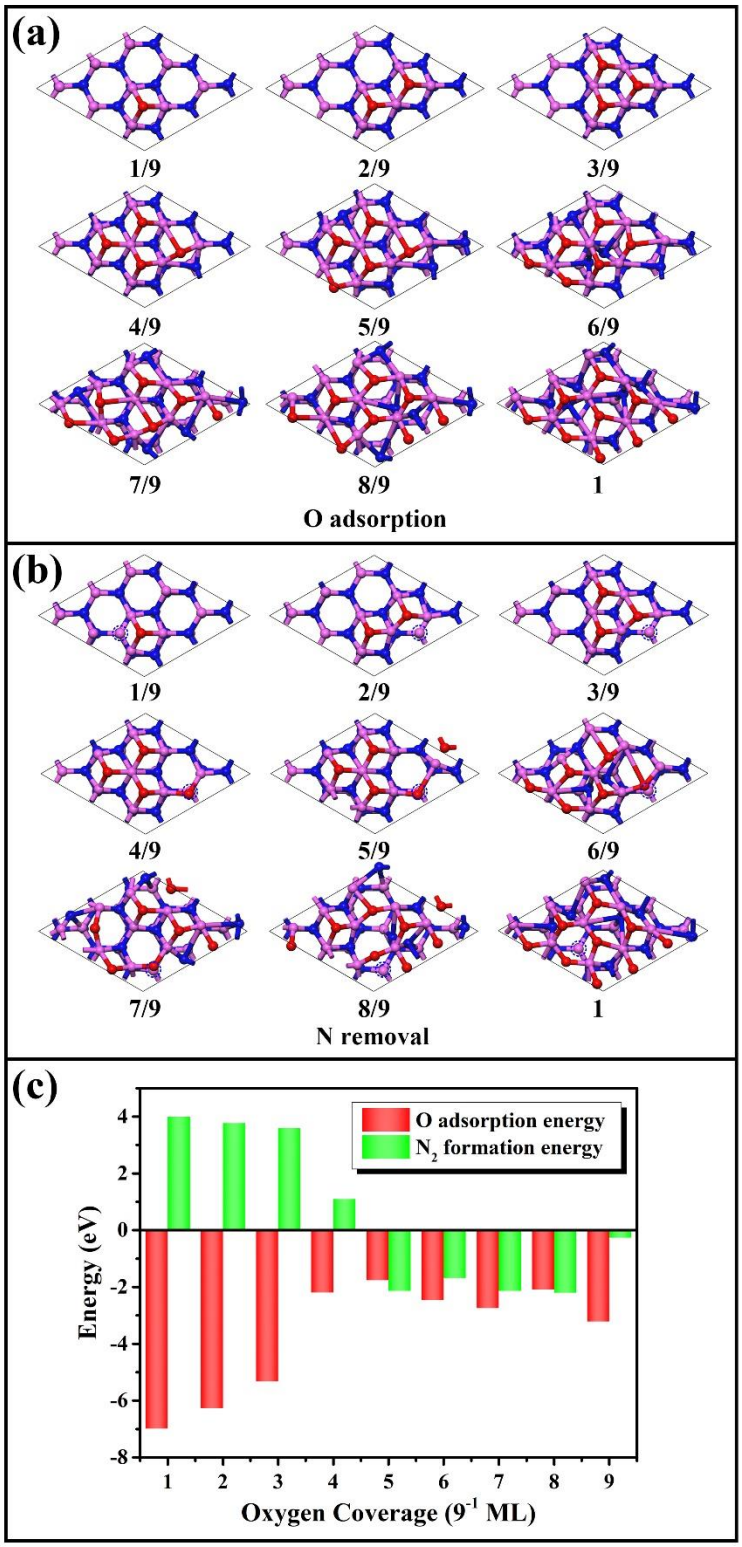

Figure S1. Optimized structures after (a) adsorption of O and (b) emission of N_2 at different oxygen coverages (ranging from 1/9 to 1). (c) Adsorption energies of O adsorption and formation energies of N_2 emission. Removed N atoms are labeled by dashed blue circles.

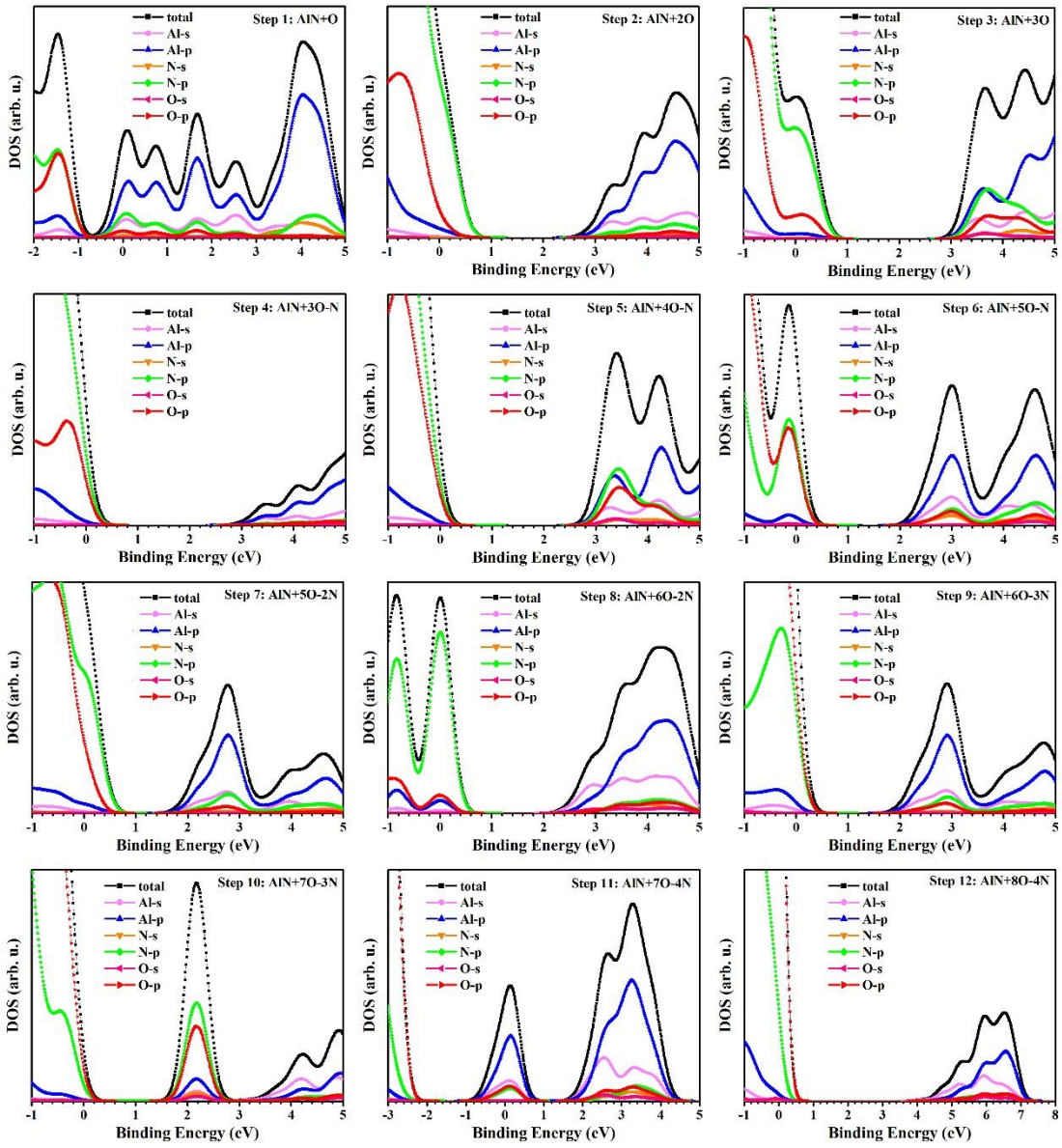

Figure S2. Total and partial density of states for *s* and *p* orbitals of each element on the AlN (0001) surface in every step of the oxidation process.

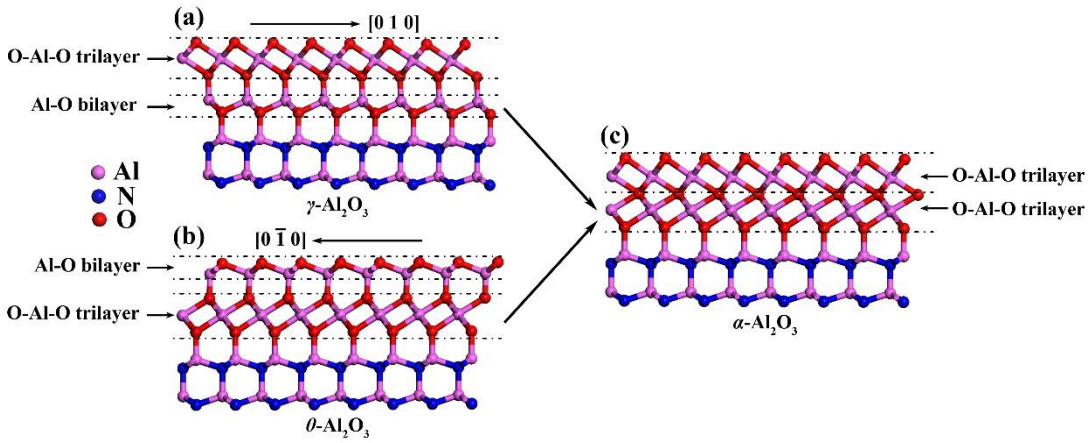

Figure S3. Models of the AlN surface with (a) γ-Al_2O_3-like (b) θ-Al_2O_3-like and (c) α-Al_2O_3-like oxide layers. Models a and c are simulated structures in our work and Model b is quoted from Reference 6.