

Adsorption mechanisms of decomposition species of CHON-containing explosives on aluminum surfaces

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Supporting Information (SI)

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S1. Density of states (DOS) distributions of the Al surfaces before and after adsorbing different species.

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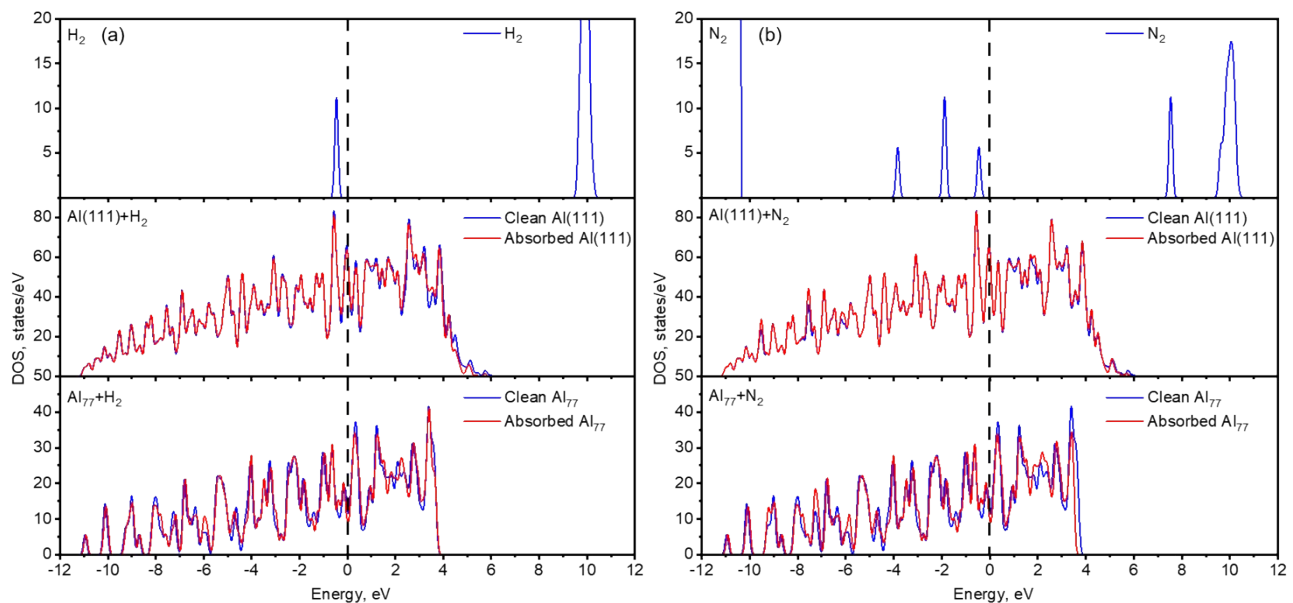


Fig. S1 DOSs of different Al surfaces before and after adsorption of H_2 (a) and N_2 (b), and DOSs of corresponding free molecules are also plotted in the top of figure. The dashed line represents the Fermi level. This representation is also employed in following figures.

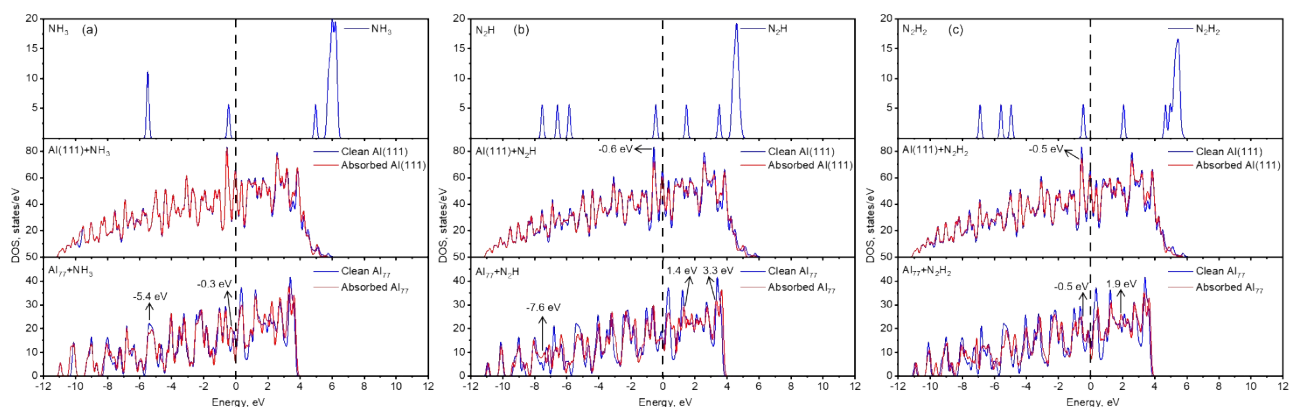


Fig. S2 DOSs of different Al surfaces before and after adsorption of NH_3 (a), N_2H (b) and N_2H_2 (c). The arrow indicates the positions of the DOS peaks change on the adsorbed Al surface compared to the clean surface.

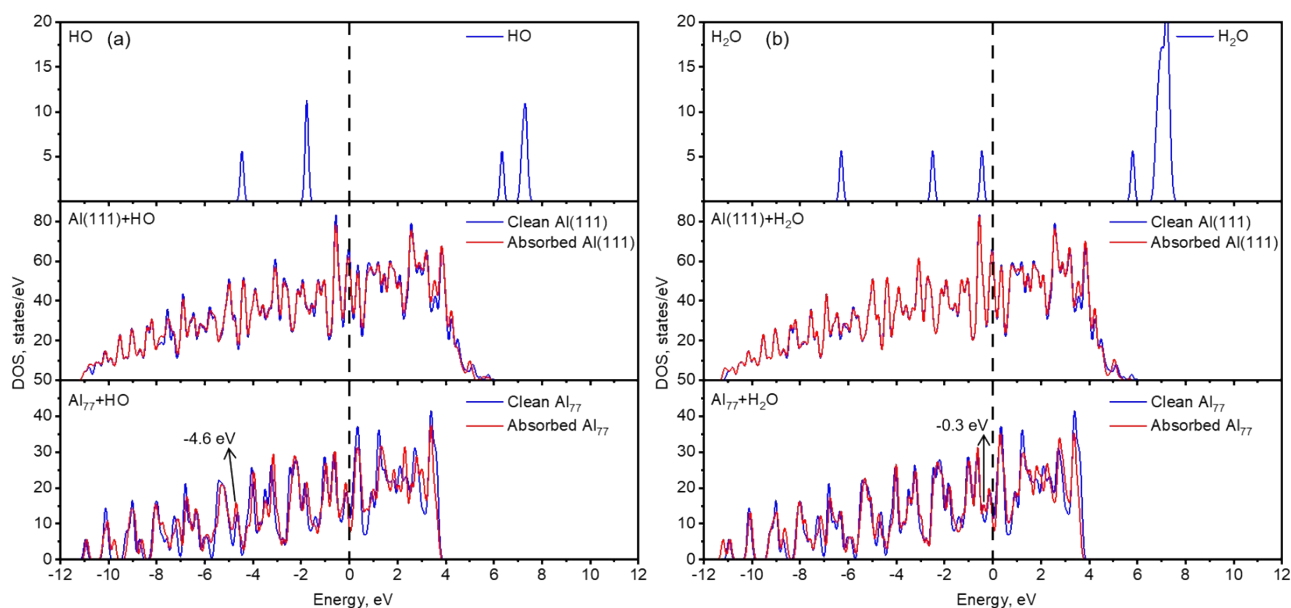


Fig. S3 DOSs of different Al surfaces before and after adsorption of HO (a) and H₂O (b).

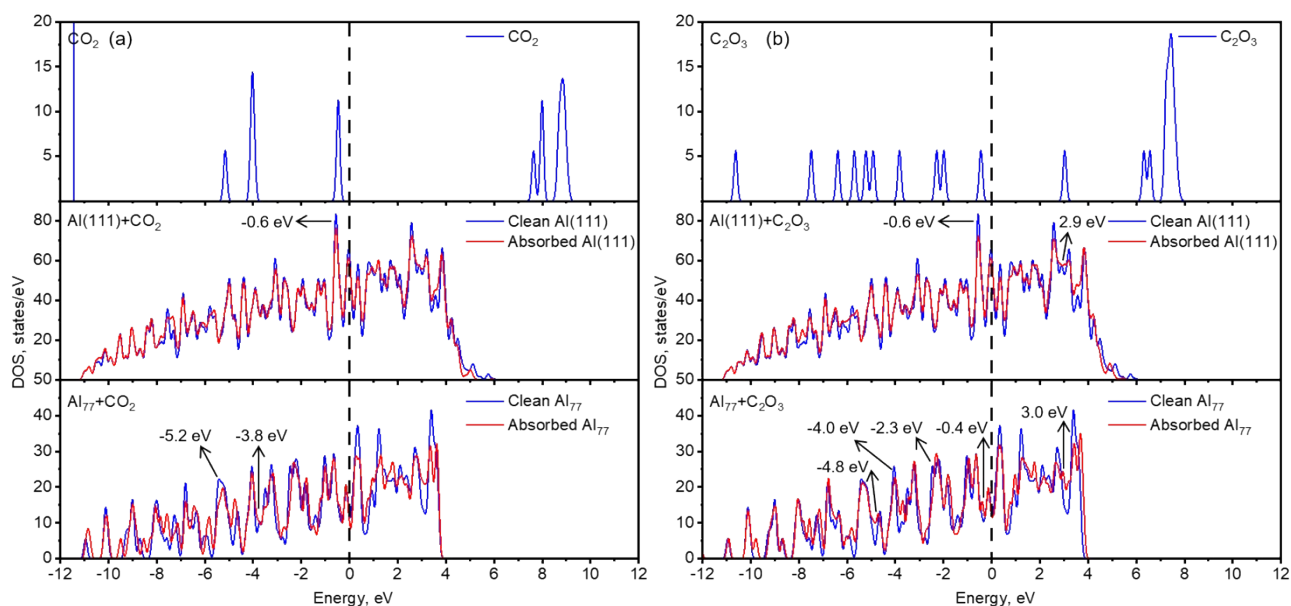


Fig. S4 DOSs of different Al surfaces before and after adsorption of CO₂ (a, b) and C₂O₃ (c, d).