Catalytic Dehydrogenation of Propane: The Role of Chromium-Supported on Transition-Aluminas

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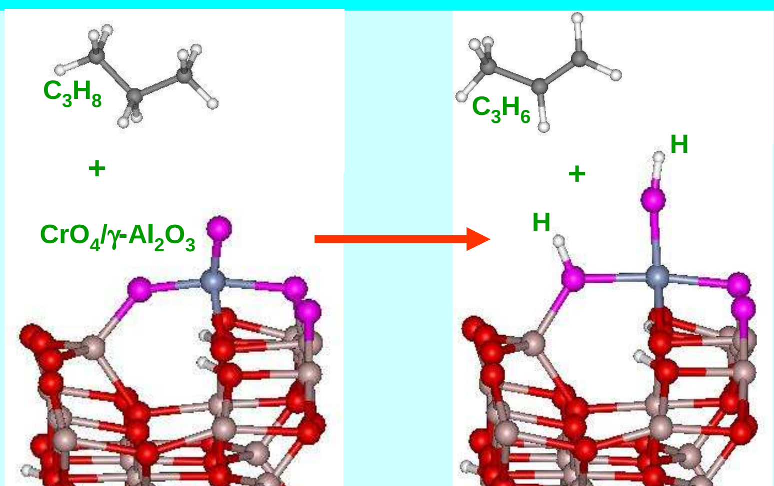
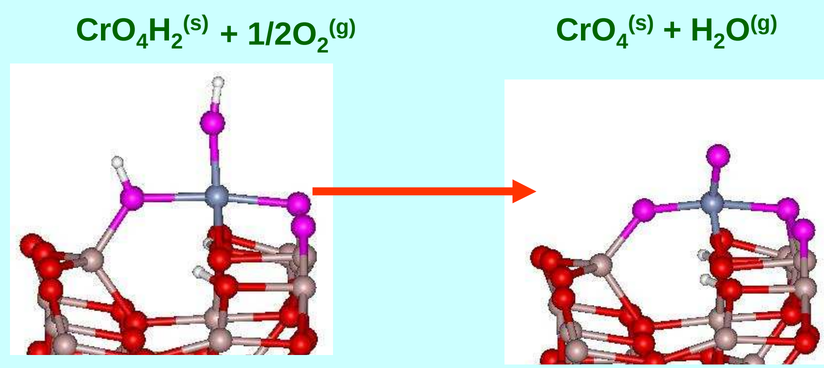
Chromium/transition-aluminas are well-known catalysts in petrochemical industry for the production of alkenes via dehydrogenation of alkanes. However, the question about the specific role of Cr/transition-aluminas in the pertinent reactions still remains open.

First-principles quantum mechanical calculations for the catalytic chemical reaction of the dehydrogenation of a selected alkane, propane (C_3H_8), with the presence of Cr (in the form of dispersed chromium oxide species) supported on γ-alumina (γ-Al_2O_3) have revealed the atomic-scale mechanism of the reaction and the role of the catalyst.





Dissociation of C_3H_8: The key step of the dehydrogenation in the presence of a CrO_4 species supported on γ-Al_2O_3.

-- Propene (C_3H_6) is released via dissociation.

-- Two hydrogen atoms of propane are trapped at the oxygen sites of the Cr oxide species.

-- The process is energetically favorable (energy gained: 0.2 – 1.6 eV).

De-hydration of CrO_4H_2: The step necessary for Cr oxide to regain its catalytic activity.

-- “Hydrated” oxygen sites are catalytically inert.

-- A flow of oxygen molecules removes the two hydrogen atoms and releases one water molecule.

-- The process also gains an energy (0.6 – 1.9 eV).