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Interaction of atomic hydrogen with FeO(111), Fe_3O_4(111) and alpha-Fe_2O_3(0001-biphase) surfaces

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Hematite Fe_2O_3 is used as catalyst in the dehydrogenation of ethylbenzene to styrene. The formed hydrogen reduces the oxide but little is known about the the mechanism. Therefore, the interaction with molecular and atomic hydrogen and its desorption was studied on epitaxial iron oxide films of different phases using LEED, XPS and TDS. Room temperature exposure to atomic H causes partial disordering. Both OH groups and reduced (but not yet metallic) iron appear in XPS. FeO domains react very quickly and TDS shows only water desorption explaining the observed reduction. Fe_2O_3 domains react more slowly. Even at RT, Fe_3O_4 domains are formed. TDS shows desorption of both H_2O and H_2. Upon flashing, reduced iron and OH remain but the oxide reorders and separates into Fe_2O_3 and Fe_3O_4. Oxidation restores the original surface. The implications for the behavior of the catalyst will be discussed.

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