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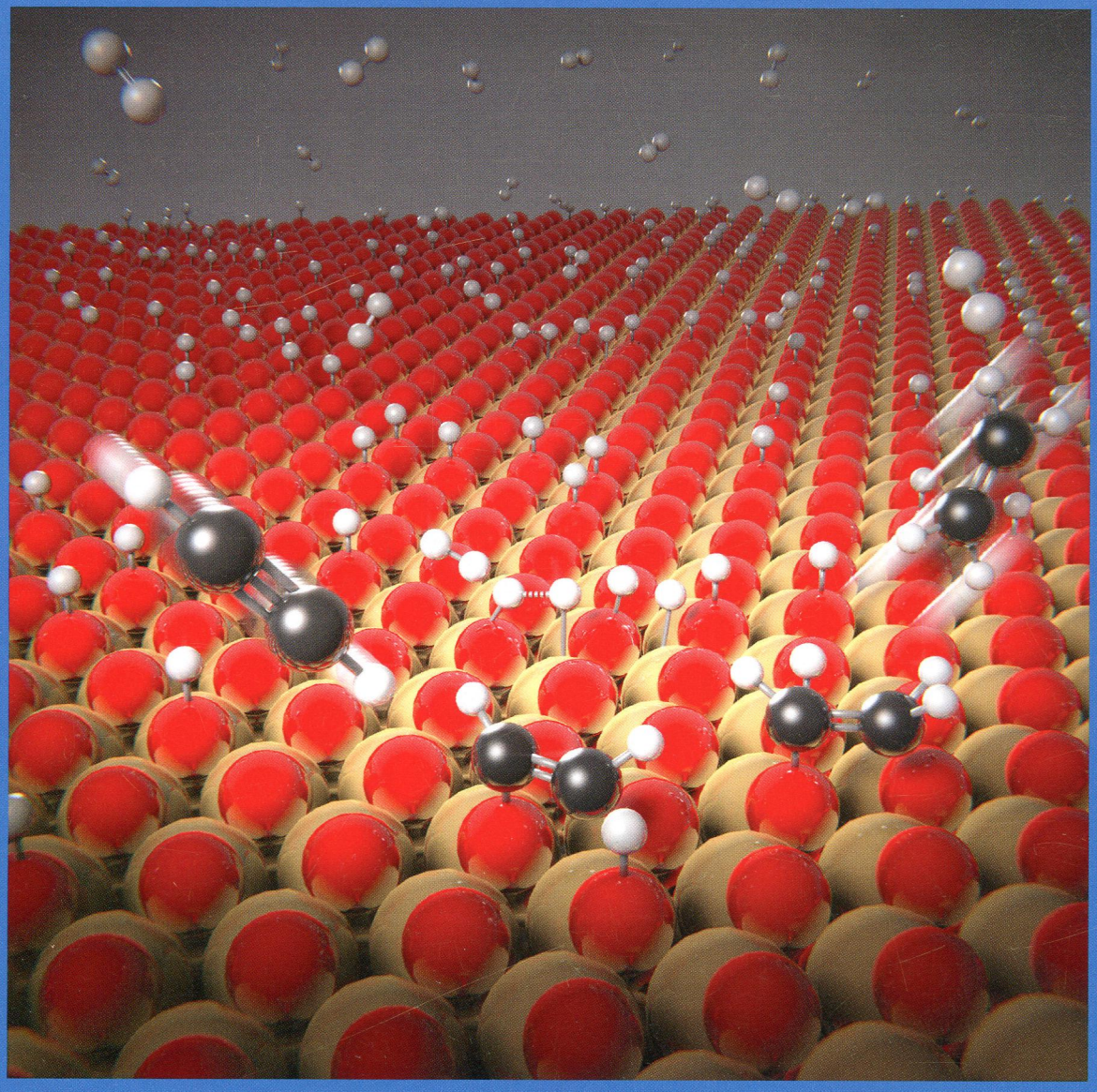

The Hydrogenation Playground on Ceria
(see page 5352)

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ON THE COVER: The hydrogenation playground on ceria. Ceria is a key component in many heterogeneous catalysts. In typical applications, ceria magnifies the performance of the active phase, but the stand-alone catalytic function of ceria is rare and usually related to oxidations. Interestingly, we reported an unprecedented performance of pure ceria for the partial hydrogenation of acetylene to ethylene with outstanding selectivity. Experimental evidence shows that (111) facets are especially prone to hydrogenation. We combine in-depth characterization, catalytic tests, and density-functional theory mechanistic studies to provide a molecular-level understanding of the hydrogenation of acetylene on the $CeO_2(111)$ surface. Acetylene adsorption leads to the formation of highly reactive C_2H_2 radical species that are hydrogenated to form C_2H_3 with no barrier at large H_2/C_2H_2 ratios. The high alkene selectivity is owed to the lower activation barrier for subsequent hydrogenation, leading to gas-phase ethylene compared with that for the formation of adsorbed C_2H_4 radical species that would enable complete hydrogenation. Our results open exciting perspectives for investigating the ability of pure ceria as a catalyst for the selective hydrogenation of alkynes and other functional groups. Cover art was created with the help of Enrique Sahagún (www.scixel.es). See page 5352.

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