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Theoretical Insights into C1 Surface Chemistry

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Reforming and partial oxidation of methane as well as other C1 fuels are important processes in the production of hydrogen and synthesis gas and will likely play important roles future energy strategies. Herein we use theory and simulation to examine the reactivity of methane, methanol and dimethyl ether with CO_2, H_2O, or O_2 over supported transition metals. We systematically probe the elementary C-H bond activation as well as the oxidation pathways involved in both reforming as the oxidation of methane and other C1 intermediates over well defined transition metal surfaces, metal alloys and metal nanoparticles. The calculations demonstrate well-established trends in C-H bond activation as the result of changes in the metal, the activating molecule (methane, methanol, and DME) as well as the reaction conditions. The reaction conditions ultimately dictate the surface coverage of carbon and oxygen which have important consequences on the surface reactivity. The theoretical and simulation results are compared with well defined experiments carried out at Berkeley over supported particles.