

Dissociative adsorption of methane on flat and stepped surfaces

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In this talk I will summarize recent Density Functional Theory (DFT) and quasi-classical trajectory (QCT), supersonic molecular beam (SMB), and reflection absorption infrared spectroscopy (RAIRS) results in connection with methane dissociative adsorption on flat and stepped surfaces: Pt(111), Ir(111), Pt(110)-(2x1), and Pt(211). The most relevant mechanisms responsible for the first bond scission of methane upon adsorption, as a function of the initial impact energy and vibrational state of the molecule will be discussed in detail, as well as the origin of the prominent role of surface temperature under conditions close to those of real catalysis. The active role of low-coordination metal atoms will be also illustrated in the case of stepped-like surfaces. Last but not least, the site-dependent stability of the formed methyl group post dissociation in the case of surfaces exposing steps and facets will be also addressed.