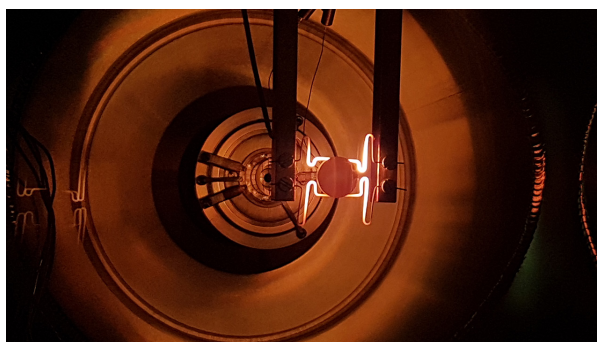


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Surface investigations take steps toward controlling gas/surface reactions on a catalyst surface

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A combination of measurement techniques reveals site-specific gas/surface interactions of complex surfaces, providing detailed reaction dynamics data to inform theoretical models.



To design optimal catalysts for chemisorption reactions, important in industrial catalysis, theoretical models still need refining to reliably predict gas/surface reactions. Recent studies show that the reactant vibrational state determines which bonds are cleaved during chemisorption reaction – so-called bond selectivity. Gutiérrez-González et al. sought to further elucidate bond selectivity for methane gas exposed to different sites on a catalyst's surface. By combining laser spectroscopy, molecular beam scattering, and infrared spectroscopy, they simultaneously probed both bond- and site-sensitivity of methane dissociation on a Pt surface.

The authors investigated two different types of bond cleavage, C-H or C-D, using deuterated methane (CH_3D). The platinum surface had two types of reactive sites for investigation: terraces and steps. Reflection absorption infrared spectroscopy detected different dissociation products and distinguished the site of chemisorption, and a quantum state resolved molecular beam was aimed at the Pt(211) surfaces in an ultrahigh vacuum chamber.

The group performed experiments with different beam incident speeds, with or without vibrational energy transferred to a specific bond via infrared laser pumping technology. Both types of sites displayed bond selectivity, with higher reactivity confirmed on the steps. Quantification showed that with increasing incident speed, the bond selectivity switched from steps to terraces, and that bond, as well as site, selectivity could be controlled by tuning translational and vibrational energies.

The authors are passing their experimental findings on to theorists across the world to aid in their development of predictive models for chemisorption reactions, and now want to examine yet another kind of surface defect sites – kinks – where two rows of steps meet. “Real catalysts are composed of a number of different sites and the goal is to study all those sites separately, and then see if we can understand them in the real metal nanoparticles used in industry,” said co-author Rainer Beck.

Source: “Bond selective dissociation of methane (CH_3D) on the steps and terraces of Pt(211),” by Ana Gutiérrez-González, F. Fleming Crim, and Rainer D. Beck, *Journal of Chemical Physics* (2018). The article can be accessed at <https://doi.org/10.1063/1.5041349>.

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