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Abstract for an Invited Paper
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Molecular Factors Determining Selectivity in Catalysis.¹

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Achieving high selectivities is arguably the main challenge in heterogeneous catalysis for the 21st century. In complex reaction with competing parallel pathways, small changes in the relative values of the different activation energies are sufficient to switch the selectivity of those processes from one product to another. We in our laboratory have been carrying out mechanistic studies on model metal surfaces to try to identify the key factors that control such selectivity. In this talk we will present several examples of increasing subtlety from that work, with focus on the conversion of hydrocarbons. Specifically, we will discuss issues of regioselectivity and stereoselectivity in early dehydrogenation steps, and how those affect selectivity in the conversion of olefins. Time permitting, we will also discuss issues related to the bestowing of enantioselectivity on solid surfaces.

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