The weird and wonderful World of Catalysis and how I got there

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Catalysis is at the heart of chemical science and is key to the development of an environmentally friendly chemical industry, yet the workings of many key industrial heterogeneous processes like the Haber-Bosch production of ammonia are poorly understood. This is the result of a gap that has so far existed between the low temperature regime at which experiments and theoretical investigations have been feasible and the high temperature and high pressure operando conditions. This gap is being closed more slowly by experiments and more quickly by theory. Progress in theory has been fueled by the application of machine learning methods to *ab-initio*-like molecular dynamics simulations. These simulations have revealed a very complex behavior in which the presence of the reagents modifies not only the surface structure but sometimes also the bulk. An industrial catalyst is not just a support for active sites but is transformed by temperature and reagents into a highly fluctuating state of matter in which active sites are continuously formed and destroyed, thus avoiding poisoning. We shall also review from a personal perspective the complex and long pathway that has enabled addressing such a complex problem.