"Complexity" in dissociative adsorption of "simple" molecules on metal surfaces

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Abstract:

Since mid-90's we have been witnesses of a tremendous advance of the comprehension of reactive adsorption processes at surfaces thanks to the development of new methods and algorithms and the increase of computational power which today allow accurate dynamical descriptions from first principles. However, most of the theoretical dynamics studies based on precise interaction potentials obtained from Density Functional (DF) calculations have dealt with diatomics and "simple" flat, homogeneous (mono-metallic) and clean surfaces. In this talk we will analyze, through a few selected examples, the role in the dissociative adsorption process of the "complexity" introduced by: i) preadsorbed species (coverage effects), ii) metal atoms "decorating" simple surfaces, and iii) higher atomicity of the molecules. DF and DF-based classical trajectory results will be presented with this aim, and also to illustrate some possibilities and limitations of state-of-the-art dynamical simulations.