Defects in 2D Materials & Single Atoms on Oxide Surfaces: possible catalysts for a sustainable future

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In the pursuit of a sustainable future, the last decade has seen a concerted effort in accelerating the discovery of materials for energy needs, thanks to the Materials Genome Initiative which has facilitated close collaboration between experiment, theory, modeling, and simulation. In this talk I will focus on a few low-dimensional materials which provide opportunities for tailoring their chemical properties for potential application as catalysts for technologically relevant processes such as CO and CO_2 hydrogenation and NH_3 oxidation. I will show how defects and dopants in single-layer MoS_2 convert it into a cheap catalyst for CO hydrogenation[1]. Even more interesting is the case of another 2D material, hexagonal boron nitride (*h*-BN), a well-known insulator. Defects can transform *h*-BN to a metal-free catalyst that captures and converts CO_2 to value added products such as methanol[2]. Further opportunities for tuning of the local environment are provided by singly dispersed Pt or Pd atoms on ceria, with or without the help of ligands. I will show how depending on the local environment Pt atoms on ceria serve as excellent catalysts for either CO or for NH_3 oxidation.[3] Ligands can also play an important role in controlling reaction thermodynamics and kinetics, as shown for singly dispersed Pd atoms on ceria.[4] With a focus on electronic structural modulations of the local environment, I will draw comparisons with experimental observations made in collaborative research, and point to some factors that could serve as descriptors of the active site.

[1] D. Le, T. B. Rawal, and T. S. Rahman, J. Phys. Chem. C 118, 5346 (2014); T.B. Rawal, et al., J. Chem. Phys. 154, 174701 (2021).

[2] K. Chagoya, et al., ACS Sustainable Chem. Eng. 9, 2447 (2021); T. Jiang, et al., Phys. Chem. Chem. Phys. 23, 7988 (2021).

[3] W. Tan, et al., Nat Communications 13, 7070 (2022)

[4] E. Wasim, et al., J. Catalysis 413, 81 (2022)