Interfacial Phenomena in Heterogeneous Catalysis

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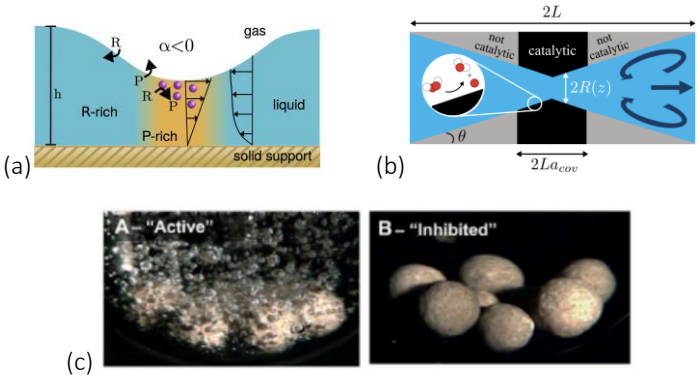

Figure 1: a) Marangoni flows in thin reactive films [1] b) Diffusio-phoretic pumping in catalytic pores [2] c) Inhibition of LOHC dehydrogenation due to capillary trapping of hydrogen [3].

Interfacial phenomena play an important role in heterogeneous catalysis, influencing the efficiency and selectivity of catalytic processes. They can significantly alter the transport of reactants, especially in multiphase systems. On top of that, catalytic "hotspots" generate local chemical gradients, that can trigger flows and instabilities at the interfaces and can affect the behavior of the system at larger scales. Our group uses simulations (Lattice-Boltzmann method) and theoretical tools to study these phenomena at micro- and macroscale. In particular, we study instabilities induced by Marangoni flows in thin chemically reactive films, which can lead to film de-wetting [1], spontaneous generation of diffusio-phoretic flows in pores with catalytic hotspots, which can enhance mixing at the pore scale [2], inhibition of dehydrogenation of liquid-organic hydrogen carriers (LOHCs) due to capillary trapping of hydrogen in porous catalyst [3,4], highly selective transport of reactants in porous catalysts, leading to tunable selectivity for competing chemical reactions [5].

[1] T.Richter et al. arXiv preprint, arXiv:2402.14635 (2024).
[2] G. Antunes et al. Phys. Rev. Lett, (2022), *129*(18), 188003.
[3] T.Solymosi et al. Science Adv. (2022), 46(8), eade3262.
[4] T. Nizkaia et al., in preparation
[5] T. Nizkaia et al., in preparation .