Tailoring the Selectivity of 1,3-Butadiene versus 1-Butene Adsorption on Pt(111) by Ultrathin Ionic Liquid Films

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Ionic Liquids (ILs) – low melting salts with melting points typically below 100 °C have promising applications in catalysis. Particularly, the Solid Catalyst with Ionic Liquid Layer (SCILL) concept proved to enhance the selectivity of hydrogenation reactions, like the selective hydrogenation of 1,3-butadiene to 1-butene using transition metal catalysts. In this context, the adsorption dynamics of 1,3-butadiene and 1-butene were studied on Pt(111) modified with ultrathin layers of the IL 1,3-dimethylimidazolium bis(trifluoromethanesulfonyl)imide ($[C_1C_1Im][Tf_2N]$).

We will show sticking coefficient measurements of the two olefins using the direct method of King and Wells. Both olefins show pronounced precursor-mediated dynamics on clean Pt(111) and on the IL-modified surface. Increasing the IL coverage leads to an increased blocking of adsorption sites for the incoming olefins. Interestingly, a smaller IL amount is needed to prevent 1-butene adsorption as compared to 1,3-butadiene adsorption (see Fig. 1), which we propose to be directly related to the IL's influence on selective hydrogenation in SCILL catalysis.

With the help of our molecular dynamics simulations, we will show that IL film densification/relaxation is the key mechanism to allowing/excluding olefin adsorption on the metal. Being a function of IL coverage, the energy of film penetration determines the effective olefin adsorption energy – and thus creates an operation regime for suppressing 1-butene while permitting 1,3-butadiene adsorption.

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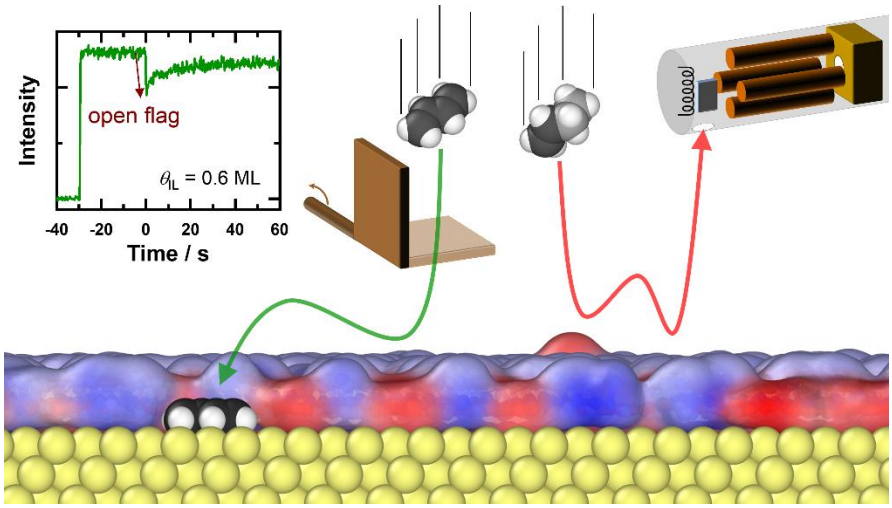

Fig. 1. In a higher IL coverage regime, 1,3-butadiene adsorption is measurable, while 1-butene adsorption is suppressed. Molecular dynamics simulations show that depending on the olefin a different amount of energy is required for IL film densification.