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Impact of interfacial solvent restructuring onto catalytic behavior by PDF

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Noble metal nanoparticles (NP) play a major role in modern heterogeneous catalysis. Reaction conditions like temperature and pressure impact the catalytic activity and selectivity. [1] Although a solvent effect is commonly accepted as a decisive parameter in liquid-phase catalysis, its fundamental understanding on a molecular level is still missing. Pair distribution function (PDF) analysis based on high-energy X-ray scattering experiments can access the size of and the molecular ordering within solvation shells around colloidal NPs. [2] To correlate solvent-dependent catalytic activity with the interfacial solvent structure, we performed the selective hydrogenation of styrene to ethylbenzene under atmospheric hydrogen pressure in various organic solvents like tetrahydrofuran (THF) and toluene. Dodecanethiol stabilized palladium (Pd) NPs with an average diameter of 3 nm acted as catalyst. The difference-PDF signal of the THF dispersions reveals four restructured layers of THF molecules stretching 2 nm away from the NP surface. Corresponding catalytic studies (gas chromatography) allow a structure-activity correlation. Finally, GC-MS can be coupled to in-operando PDF measurements (1 min time resolution) to track structural changes of both NP and interfacial solvent layers in liquid-phase catalysis.

[1] U. K. Singh et al., Appl. Catal., A 2001, 213, 1

[2] Zobel, M. et al., Science 2015, 347, 292

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