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ABSTRACT

The liquid-phase hydrogenation of phenylacetylene (PA) over 1 wt.% Pd/Al_2O_3 catalysts with the mean palladium cluster size varying from 1.5 to 22 nm was studied at 5 bar H_2 pressure and 25^{o}C. Turnover frequency in hydrogenation of the triple and double bonds displayed a significant increase with an increase of the cluster size, which was more pronounced for the former case.

The effect of Pd nanoparticle size on the hydrogenation kinetics was analyzed and discussed using an approach based on a continuous distribution of edges and terraces exhibiting different reactivity. A quantitative description of the concentration dependences with incorporation of Pd particle size in the rate equations demonstrated an excellent correspondence between theory and experiments.

Key-words: structure sensitivity, hydrogenation of phenylacetylene, palladium, kinetic modelling