



Active Sites in Heterogeneous Catalysis

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Message from the Guest Editor

Knowledge of the structure and composition of active sites is crucial to understand heterogeneous catalysts and design more efficient ones. This is particularly true since the scarcity of some elements such as noble elements widely used in energy and environment fields will require doing better with less. As suggested by Taylor in 1925, active sites are considered as atoms or ensembles of atoms sparse on the surface which directly catalyze a reaction. Active sites change in a dynamic way during adsorption of reactants or reaction intermediates, and this dynamic restructuring plays an important role in bond activation. Detailed description of active sites using advanced in situ/operando techniques with high temporal and spatial resolutions as well as DFT modeling allow establishing structure–activity relationships. They are particularly interesting for single atoms and subnanometric clusters, which can be distinguished by the atomically resolved microscopes.

