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Identification and optimisation of active electrocatalytic sites for fuel cell applications

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According to the existing paradigms of heterogeneous catalysis, the first steps in the design of new catalysts consist of two procedures: identification of the nature of so-called active sites (after H.S. Taylor, 1925) and their optimization, so that they bind reaction intermediates optimally (P. Sabatier, 1911). In contrast to homogeneous catalysis, where the methodology of elucidating the active sites is rather developed, heterogeneous (electro)catalysis suffers from the absence of well-established means to find them at the surface. Namely the lack of understanding of the nature of the catalytic centers largely hinders further optimization of their electronic properties and hence their activity, selectivity and stability. In the presentation, several experimental and joint theoretical/experimental approaches will be presented in order to identify active sites and design new better materials for the fuel cell applications. One example is illustrated in Figure 1, where theoretical analysis and experiments with model "stepped" single crystals explain the high activities of the "concave" nanoparticles towards the oxygen reduction reaction (ORR).

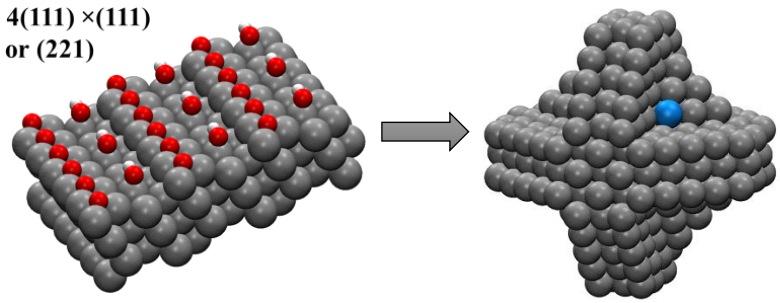

Figure 1: Joint theoretical and experimental identification of the nature of active catalytic sites helps in rational design of improved nanostructured electrocatalysts [1]. For instance, the most active towards the oxygen reduction reaction sites of Pt materials are located at the "concave" sites [2]. Adapted from [2].

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