Fast and rational design of multifaceted catalysts by means of structure-sensitive scaling relations

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Catalysis plays a prominent role in society, as it enables the production of countless chemical compounds and promises future clean and reliable energy solutions. However, numerous catalytic reactions are currently inefficient. Scaling relations between adsorption energies simplify the computational design of catalysts [1], as they have only two parameters: a slope and an offset [2-3]. However, they are currently restricted to low-index surfaces, so they cannot fully describe real multifaceted catalytic surfaces.

Here we incorporate structure sensitivity in scaling relations by examining the adsorption energies of *O and oxygenates (*OR = *OH, *OOH, *OCH₃) on twelve different facets of nine transition metals [4]. The resulting scaling relations show that the slope depends on electron-counting rules on the adsorbates and is surface independent [2-4]. Conversely, the offset depends on the coordination number of the surface [4]. Therefore, structure-sensitive scaling relations can be rapidly predicted using simple electron and nearest-neighbor counting rules and be used for the rational computational design of the composition and morphology of optimal catalysts.