



Preface to the Special Issue on Single Atom Catalysis

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Abstract

This special issue contains articles that aim to determine the structure and mechanisms underlying single-atom catalysis.

The field of single-atom catalysis (SAC) has exploded over recent years, and is now firmly established as a major focus of thermal-, electro- and photocatalysis research. Although this recent explosion was largely motivated by minimizing the amount of precious metal required for heterogeneous catalysis, it is now clear that SAC systems can exhibit higher turnover frequencies than metal nanoparticles in some reactions, can exhibit unique selectivities, and might even provide the long-sought after bridge between heterogeneous and homogeneous catalysis.

The recent rise of SAC research, particularly work focused on late-transition metals, came about following dramatic advances in the resolution of transmission electron microscopy (TEM) in the 2000s. Suddenly, it became possible to visualize single atoms on a catalyst support, and it was confirmed that single atoms often coexist with the metal nanoparticles. Suspicions that the single atoms might be (partly) responsible for catalytic activity led to attempts to synthesize catalysts featuring single atoms only, and it has now been established that such systems can exhibit superior performance in some cases. The key difference between single atoms and metal nanoparticles originates in the electronic structure, because single atoms exchange electrons with the support when they form chemical bonds. These characteristics modify the strength of the interaction with reactants, and potential reactions between adsorbed intermediates, and thus the catalytic activity. One of the

most interesting potential consequences, however, is that the optimal metal for a particular reaction need not be the same as the established nanoparticle catalyst: cheaper, more sustainable elements might perform equally well or better. Screening through the different possibilities should be ideal territory for theory, but the conclusions depend strongly on the active site coordination and the reaction mechanism assumed. Unfortunately, this information also remains difficult to obtain from experiment, and it is not clear if what is calculated is representative of reality.

The importance of the atoms charge state and its coordination environment draws inevitable comparisons to the molecular species utilized in homogeneous catalysis. There is currently much excitement that SAC might be able to achieve similar levels of selectivity, or even be used to heterogenize reactions typically performed in solution. To achieve this lofty goal, the field must develop the ability to precisely determine the active site coordination, and to modify it to facilitate specific reaction pathways. This is the key strength of homogeneous catalysis, but it remains a significant challenge on inhomogeneous support surfaces. The dream requires further development of our experimental methods, and we must go beyond seeing the atoms to also seeing their local coordination environment and understanding how this adapts with changing environments. This is critical to forge strong links to theory, and ensure that realistic atom geometries are considered. While much research in SAC is focused on discovery (e.g. novel synthesis methods, new reactivity...), fundamental studies of structure–function relationships at the active site coordination level are critical to continue to push the field forward. In this special issue, we feature papers demonstrating the state of the art, in which understanding how the structure of the active site relates to the reactivity is the issue of paramount importance. We very much hope that the spirit of collaboration shown here can

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serve as a springboard for rapid developments in this exciting research area.

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