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Mechanistic insight towards the activation of aerobic oxidative coupling reactions of alcohols on nanoporous gold

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Bulk gold has been known as an inert material without any specific catalytic activity for almost a century. But then in the 1970s Bond et al. presented small gold particles placed on a SiO_2 support that could be used for the hydrogenation of alkenes and alkynes. Since this decade a lot of research has been done on nanostructured gold. These Au-based catalysts can be used for fuel cells, the synthesis of esters or the selective oxidation of alcohols. The selectivity of gold to partial oxidation products is higher than the selectivity of other metal catalysts, so there is a high interest in this gold based catalyst. A problem of gold nanoparticles as catalyst is that the efficiency increases if the average particle size is reduced so in most cases the major part of the surface area of the supporting material is not used for the catalytic processes. In addition to this supported forms of gold catalysts an unsupported form of gold, the nanoporous gold (np-Au), characterized by Zielasek et al. has recently attracted considerable interest due to its potential use in catalysis. Compared to support gold nanoparticles the complete entire surface of the material can be possibly usable as a catalytic material. The most prominent example for the use of np-Au as a catalyst is the selective oxidation of methanol. Although this reaction has been investigated by several groups, the origin of the catalytic activity of np-Au has not been understood completely. The main remaining question that we try to answer is the nature of the active sites of the np-Au. Within DFT (density functional theory) calculations, we describe the influence of residual silver atoms in the material and try to explain some possible pathways for the activation of oxygen, the most essential step of most of oxidative coupling reactions.

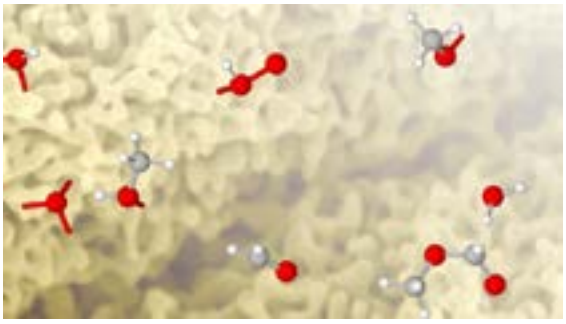

Figure 1: Possible reactant, intermediate species and reaction products for methanol oxidation on nanoporous gold.

Biography

Wilke Dononelli has his expertise in quantum chemical modeling of catalytic reactions at surfaces. In 2010, he received his Bachelor degree in Mathematics and Chemistry and he started his PhD in Theoretical Chemistry at University of Oldenburg in Germany in 2014. He has experienced in density functional theory and high level *ab initio* calculations. His main focus lies on bridging from theoretical calculations to model experiments.

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