

# From Molecular Cobalt Oxo Clusters to $\text{Co}_3\text{O}_4$ Nanoparticles: Bridging the gap between heterogenous and homogenous oxidation catalysis

T. Fockenberg<sup>1</sup>, C. Placke-Yan<sup>1</sup>, X. Ma<sup>1</sup>, S. Karwasara<sup>1</sup>, H. Amin<sup>1</sup>, S. Schulz<sup>1</sup>

<sup>1</sup>Faculty of Chemistry, University of Duisburg-Essen, Essen, Germany

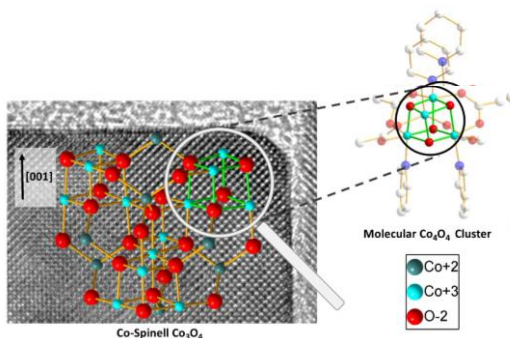
E-Mail presenting author: [timo.fockenberg@uni-due.de](mailto:timo.fockenberg@uni-due.de), [carsten.placke-yan@uni-due.de](mailto:carsten.placke-yan@uni-due.de)

To date, the detailed reaction mechanisms of metal oxide catalysts in oxidation catalysis, such as alcohol oxidation and the oxygen evolution reaction, remain unclear.

To gain further insight into these processes, nanoparticles with defined size, morphology and composition are required. Complementary, molecular models that can serve as surface cutouts allow spectroscopic *in situ* analytics such as NMR and IR. Theoretical calculations can help to interpret these results.[1]

With the here reported synthetic procedures for both cobalt nanoparticles and cobalt oxo clusters, we bridge the gap between molecular model and solid-state particle:

Cobalt nanoparticles were prepared both with different morphology[2] and composition.[3] Metal oxo clusters of different sizes were prepared with well-defined oxidation states and metal compositions. First catalytic results in oxidation catalysis will be reported for both particles and models.



**Figure 1:** Molecular  $\text{Co}_4\text{O}_4$ -Cluster as structural cutout of a cubic  $\text{Co}_3\text{O}_4$  particle with defined (001) surface termination.

[1] F. Song et al., J. Am. Chem. Soc. 2017, **139**, 14198, 10.1021/jacs.7b07361

[2] Saddeler et al., Inorg. Chem. 2020, **59**, 14, 10013, 10.1021/acs.inorgchem.0c01180

[3] Placke-Yan et al., Mater. Adv., 2024, **5**, 3482, 10.1039/D4MA00088A