Contribution ID: **244** Type: **Poster**

On the electronic and geometric structure of a single atom Cu/UiO-66 CO oxidation catalyst during reaction - An operando XAFS study

Tuesday, 18 September 2018 17:15 (15 minutes)

The single atom Cu metallated UiO-66 metal organic framework (MOF) catalyst (Cu/UiO-66) had turned out to be highly active for CO oxidation at reaction temperatures between 120 and 250℃. Combining time resolved operando XAS measurements at the Cu K-edge with operando FTIR spectroscopy, atomic resolution electron microscopy (HAADF-STEM) and DFT computations we investigated the structure of this catalyst during reaction. The measurements indicated that it reaches its highest activity after an initial activation period of 800 min, then it remains stable at extended reaction time and also under dynamic startup-shutdown operations. While XANES measurements showed that Cu exists in a composition of 30 % Cu1+ and 70% Cu2+ under steady-state conditions, EXAFS measurements indicated that Cu is predominantly bound to O, with an average coordination of 2.0 ± 0.5 at Cu-O bond distance of 1.90±0.02 Å. In agreement with these findings, electron microscopy (HAADF-STEM) indicated that Cu exists in a highly dispersed atomic state. Consequences of these findings and of additional DFT computations for the understanding of the Cu@UiO-66 structure under reaction conditions and the mechanistic understanding of these catalysts will be discussed.

References
1. H. Furukawa et al., Science 341 (2013) 1230444.
2. B. Rungtaweevoranit et al., Nano. Lett. 16 (2016) 764.

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Session Classification: Poster session 2

Track Classification: P9 Catalysis